Ukrainian Conference
with International participation

CHEMISTRY, PHYSICS
AND
TECHNOLOGY OF SURFACE

23-24 MAY 2018
KYIV
UKRAINE

National Academy of Sciences of Ukraine
Chemistry Division
Chuiko Institute of Surface Chemistry
Scientific Council
"Chemistry and Technology of Surface Modification"

Ukrainian Conference with International participation

CHEMISTRY, PHYSICS AND TECHNOLOGY OF SURFACE

Book of abstracts

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Ukraine

Матеріали Всеукраїнської конференції з міжнародною участю «Хімія, фізика і технологія поверхні» – Київ, 2018. – 190 с.

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Збірник містить тези доповідей, які було представлено на конференції. Тематика конференції: теорія хімічної будови та реакційна здатність поверхні твердих тіл; фізико-хімія поверхневих явищ; хімія, фізика та технологія наноматеріалів; медико-біологічні та біохімічні аспекти дослідження високодисперсних матеріалів. Тези доповідей подано в авторській редакції.

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Conference Program

May 23, Wednesday

9:00 – 9:45 Registration of participants

10:00 – 10:20 Opening of the Conference at the Chuiko Institute of Surface Chemistry of National Academy of Sciences of Ukraine
Academician of NAS of Ukraine, Professor M. Kartel

Oral Session 1
Chair: Professor M. Kartel

10:20 – 10:40 V.V. Turov, V.M. Gun'ko, T.V. Krupska, M.T. Kartel. **Influence of solid and liquid hydrophobic compounds on characteristics of water located in an adsorption layer of a hydrophilic component of the system** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).

10:40 – 11:00 V.M. Gun'ko. **Methods for description of the textural characteristics of various materials** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).

11:00 – 11:20 Coffee break

Oral Session 2
Chair: Professor V. Rozenbaum

11:20 – 11:40 A.N. Herega, Yu.V. Kryvchenko. **Genesis of surface films as a self-organized criticality: Computer model** (*Odessa National Academy of Food Technologies, Ukraine*).

11:40 – 12:00 S.D. Kaim. **The high-energy nanoreactors in condensed matter** (*Faculty of Electrical Engineering, Automatic Control and Informatics, Opole University of Technology, Poland*).

12:00 – 12:20 V.P. Grankin, D.V. Grankin. **Nonadiabatic chemoelectron conversion of the energy of interaction of gas particles with surface** (*Pryazovskyi State Technical University, Mariupol, Ukraine*).

12:20 – 12:35 S.M. Duvanov, S.N. Danilchenko. **Nanocrystallite growth activation energies of the apatite under isochronal thermal treatment** (*Institute of Applied Physics, NAS of Ukraine, Sumy*).

12:35 – 12:50 A. Ievtushenko[1], V. Karpyna[1], O. Bykov[1], O. Kolomys[2], S. Mamykin[2], O. Olifan[1], V. Baturin[3], O. Karpenko[3], V. Strelchuk[2], G. Lashkarev[1]. **The effect of substrate bias on structure, optical and electrical properties of wide bandgap oxides films** (*[1]Frantsevich Institute for Problems of Material Science, NAS of Ukraine, [2]V. Lashkarev Institute of Semiconductor Physics, NAS of Ukraine, Kyiv, [3]Institute of Applied Physics, NAS of Ukraine, Sumy*).

12:50 – 13:05 G.V. Lisachuk, **R.V. Kryvobok**, Y.M. Pitak, O.M. Lapuzina, N.A. Kryvobok, N.S. Maystat. **Radio-absorbing materials with adjustable dielectric properties** (*National Technical University "Kharkiv Polytechnic Institute", Ukraine*).

13:05 – 14:00 Break

Oral Session 3

Chair: ***Dr. (Chem.) N. Vlasova***

14:00 – 14:15 **H.V. Vasylyeva**[1], S.I. Trofymenko[2]. **The application of kinetic models to the description of sorption of strontium ions onto inorganic sorbents** ([1]*Department of Physics of Nuclei and Elementary Particles, Uzhgorod National University, Ukraine,* [2]*Institute for Sorption and Endoecology Problems, NAS of Ukraine, Kyiv*).

14:15 – 14:30 **O.I. Oranska**, Yu.I. Gornikov. **Complex X-ray diffraction and thermal analysis of bentonite clays** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).

14:30 – 14:45 **L.M. Soldatkina**. **Adsorption removal of dyes from aqueous solutions using low cost adsorbents based on agro-industrial waste products** (*Odessa I.I. Mechnikov National University, Ukraine*).

14:45 – 14:55 **M. Sęczkowska**[1], D. Sternik[1], A. Deryło-Marczewska[1], A.W. Marczewski[1], V.M. Gun'ko[2]. **Influence of structure and properties of active carbons on dyes adsorption – equilibrium and kinetics** ([1]*Faculty of Chemistry, Maria Curie-Sklodowska University, Lublin, Poland,* [2]*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).

14:55 – 15:05 **O.O. Siryk**[1], A.K. Trofimchuk[2]. **Supramolecular sorbents based on silica gels and crystalline cellulose modified with polyhexamethyleneguanidines** ([1]*F.D. Ovcharenko Institute of Biocolloid Chemistry, NAS of Ukraine, Kyiv,* [2]*Taras Shevchenko National University of Kyiv, Ukraine*).

15:05 – 15:15 **M. Goliszek**, M. Sobiesiak, K. Fila, B. Podkościelna. **The application of polymeric microspheres with lignin in sorption processes** (*Faculty of Chemistry, Maria Curie-Skłodowska University, Lublin, Poland*).

15:15 – 15:25 **R.V. Horda**[1], A.K. Trofimchuk[2], O.V. Legenchuk[1]. **Sorption of noble metals on surface silica gel and phytosorbents with chemical grafted thiourea groups** ([1]*F.D. Ovcharenko Institute of Biocolloidal Chemistry, NAS of Ukraine, Kyiv,* [2]*Taras Shevchenko National University of Kyiv, Ukraine*).

15:25 – 15:35 L.M. Soldatkina[1], **V.O. Novotna**[1], T.V. Tiutiunnyk[1], A.P. Polikarpov[2]. **Application of response surface methodology for optimization of anthocyanin removal from chokeberry extracts by fibrous cation exchanger FIBAN K-1** ([1]*Faculty of Chemistry, Odessa I.I. Mechnikov National University, Ukraine,* [2]*Institute of Physical Organic Chemistry of National Academy of Sciences, Minsk, Belarus*).

15:35 – 15:45 **M. Samsonenko**[1], O. Zakutevskyy[1], S. Khalameida[1], J. Skubiszewska-Zieba[2]. **Study of the physical-chemical and sorption properties of SnO_2 prepared by mechanochemical and microwave routes** ([1]*Institute for Sorption and Problems of Endoecology, NAS of Ukraine, Kyiv,* [2]*Faculty of Chemistry, Maria Curie-Skłodowska University, Lublin, Poland*).

15:45 – 16:05 Coffee break

16:05 – 17:00 ***Poster session I (1-64)***

May 24, Thursday

Oral Session 4
Chair: Professor V. Gun'ko

10:00 – 10:15 **E.M. Demianenko**, V.V. Lobanov, O.S. Karpenko, A.G. Grebenyuk, M.T. Kartel. **Influence of nitrogen atoms introduced into the graphite-concrete carbon nanocluster on the H_2 adsorption** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).

10:15 – 10:30 V.A. Basiuk[1], D.E. Tahuilan-Anguiano[1], O.Yu. Tsuvariev[2,3], **T.Yu. Gromovoy**[4]. **Complexation of proteins with crown ether-functionalized fullerene?** ([1]*Instituto de Ciencias Nucleares, Universidad Nacional Autonoma de Mexico, Mexico,* [2]*Institute of High Technologies, Taras Shevchenko National University of Kyiv, Ukraine,* [3]*Institute of Molecular Biology and Genetics, NAS of Ukraine,* [4]*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).

10:30 – 10:45 **M. Wagner**, A. Varga, B. Abel. **Long-term stability of solid acid fuel cell electrodes** (*Leibniz Institute of Surface Engineering, Leipzig, Germany*).

10:45 – 11:00 **M.H. Hatahet**, U. Helmstadt, A. Varga, B. Abel. **Metal decorated graphene as novel electrocatalyst for solid acid fuel cells** (*Leibniz Institute of Surface Modification (IOM) / Leipzig University, Germany*).

11:00 – 11:15 **D.S. Kamenskyh**[1], V.A. Yevdokymenko[1], T.V. Tkachenko[1], D.A. Matviychuk[1], V.V. Vakhrin[2], V.I. Kashkovsky[1]. **Rice husk – bio-renewable sources for the obtaining of amorphous silicon dioxide and carbide for manufacturing different materials** ([1]*Institute of Bioorganic Chemistry and Petrochemistry, NAS of Ukraine, Kyiv,* [2]*LLC "Polycrystal", Kyiv Ukraine*).

11:15 – 11:25 **M. Bondarenko**, P. Silenko, N. Gubareni, O. Khyzhun, N. Ostapovskaya. **Synthesis of multilayer azagraphene and carbon nitride oxide** (*Frantsevich Institute for Problems of Materials Science, NAS of Ukraine, Kyiv*).

11:25 – 11:35 **D. Krötschel**[1], B. Abel[1,2], A. Varga[1]. **Metal oxide-carbon hybrid nanomaterials for stable electrocatalysis in solid acid fuel cells** ([1]*Leibniz Institute of Surface Engineering (IOM) / Leipzig University,* [2]*Wilhelm-Ostwald-Institute for Physical and Theoretical Chemistry, Faculty of Chemistry and Mineralogy, University Leipzig, Germany*).

11:35 – 11:55 Coffee break

Oral Session 5
Chair: ***Dr. (Chem.) O. Bakalinska***

11:55 – 12:10 A.I. Tripolskyi. **Fractal approach to the analysis of the kinetics of the heterogeneous-catalytic reaction** (*L.V. Pysarzhevskii Institute of Physical Chemistry, NAS of Ukraine, Kyiv*).

12:10 – 12:25 G.R. Kosmambetova. Influence of structural organization of nanophase catalysts on their selectivity in deep, selective and preferential oxidation of CO and methane (*L.V. Pisarzhevskii Institute of Physical Chemistry, NAS of Ukraine, Kyiv*).

12:25 – 12:40 A.V. Redkina, N.V. Kravchenko, N.D. Konovalova, V.V. Strelko. **Nanostructured zirconium silicates as supports of catalysts for dehydrogenation of propane into propylene** (*Institute for Sorption and Problems of Endoecology, NAS of Ukraine, Kyiv*).

12:40 – 12:50 N.V. Diyuk[1], O.V. Sachuk[2], V.O. Zazhigalov[2]. **Influence of ultrasonic and mechanochemical treatment on reducing properties of CeO_2-MoO_3 systems** (*[1]Taras Shevchenko National University of Kyiv, Ukraine, [2]Institute for Sorption and Problems of Endoecology, NAS of Ukraine, Kyiv*).

12:50 – 13:00 K. Fila, B. Podkościelna, M. Goliszek, A. Bartnicki. **Copolymerization and study of physicochemical properties of the microspheres based on aromatic thiols and DVB** (*Department of Polymer Chemistry, Faculty of Chemistry, Maria Curie-Skłodowska University, Lublin, Poland*).

13:00 – 14:00 Break

Oral Session 6
Chair: ***Professor V. Turov***

14:00 – 14:20 I.I. Gerashchenko. **Physicochemical aspects of behavior of enterosorbents in the gastrointestinal tract** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).

14:20 – 14:35 S.B. Bolshanina[1], **A.A. Yanovska**[1], I.G. Vorobiova[1], V.D. Ivchenko[2], A.G. Ableyev[3]. **Adsorption of silver ions by hydroxyapatite-alginate microspheres** (*[1]Sumy State University, [2]Sumy National Agrarian University, [3]LLC "Kusum Pharm", Sumy, Ukraine*).

14:35 – 14:50 I. Petrik[1], A. Eremenko[1], A. Rudenko[2], O. Tananaiko[3], M. Ishchenko[3]. **Dynamics of silver and copper ions release from bactericidal textiles modified by Ag and Ag/Cu nanoparticles in an aqueous medium** (*[1]Chuiko Institute of Surface Chemistry, NAS of Ukraine, [2]Institute of Urology of National Academy of Medical Science of Ukraine, Kyiv, [3]Taras Shevchenko National University of Kyiv, Ukraine*).

14:50 – 15:05 G.A. Dolynskyi, O.M. Lavrynenko, Yu.S. Shchukin. **The impact of reactive oxygen species on the surface structure of nanoceria** (*Frantsevich Institute for Problems of Material Science, NAS of Ukraine, Kyiv*).

15:05 – 15:15 **V.V. Paientko**[1], V.I. Kulikouskaya[2], E. Skwarek[3], D. Sternik[3], O.I. Oranska[1], Yu.I. Gornikov[1], A.K. Matkovsky[1], V.M. Gun'ko[1], A.V. Korobeinyk[1]. **Preparation of composite materials with nanosilica, kaolin clays, and pius pollen for cosmetic purposes** ([1]*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv,* [2]*The Institute of Chemistry of New Materials of NASB, Minsk, Belarus,* [3]*Faculty of Chemistry, Maria Curie-Skłodowska University, Lublin, Poland*).

15:15 – 15:25 P.P. Gorbyk[1], A.L. Petranovska[1], M.V. Abramov[1], S.P. Turanska[1], N.V. Kusyak[1], **N.M. Opanashchuk**[1], S.V. Gorobets[2], O.P. Dmytrenko[3]. **Synthesis and properties of magnetically sensitive nanocomposites based on magnetite and gemcitabine** ([1]*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv,* [2]*National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute",* [3]*Taras Shevchenko National University of Kyiv, Ukraine*).

15:25 – 15:45 Coffee break

15:45 – 16:45 ***Poster session II (65-127)***

17:00 Conference Closing

Poster presentation

1. Theory of Chemical Structure and Reactivity of Solid Surface

1. W. Rettig[1], A. Rothe[1], **M. Dekhtyar**[2], V. Kurdyukov[2], A. Tolmachev[2]. **Analogues of Brooker's Merocyanine with varied donor-acceptor strength** ([1]*Institut für Chemie, Humboldt-Universität zu Berlin, Germany,* [2]*Institute of Organic Chemistry, NAS of Ukraine, Kyiv*).
2. **V. Halysh**[1,2], D. Morais de Carvalho[3], A.V. Riazanova[3], B. Pasalskiy[4], M. Lindström[3], M. Kartel[2], O. Sevastyanova[3]. **Evaluation of the sorptive properties of sugarcane bagasse and straw materials for water purification** ([1]*Department of Ecology and Plant Polymers Technology, National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute",* [2]*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv,* [3]*Department of Fiber and Polymer Technology, KTH Royal Institute of Technology, Stockholm, Sweden,* [4]*Kyiv National University of Trade and Economics, Ukraine*).
3. **D.B. Nasiedkin**, A.G. Grebenyuk, Yu.V. Plyuto. **Simulation of molybdenum(VI) oxide interaction with a silica surface** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
4. **A.M. Mylin**, V.V. Brei. **Transformation of glycerol and dihydroxyacetone into ethyl lactate and lactic acid on oxide catalysts** (*Institute for Sorption and Problems of Endoecology, NAS of Ukraine, Kyiv*).
5. A.I. Kul'ment'ev, **A.Yu. Polishchuk**. **Calculation of Pourbaix diagrams for FeCrAl system within the framework of Accident Tolerant Fuels (ATF) concept** (*Institute of Applied Physics, NAS of Ukraine, Sumy*).
6. **O.V. Smirnova**, A.G. Grebenyuk, V.V. Lobanov. **Effect of doping with zirconium incorporation on the properties of defect titanium dioxide films: quantum chemical calculations** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).

2. Physical Chemistry of Surface Phenomena

7. **R.H. Amirov**, S.V. Sologub, N.V. Petrova, I.N. Yakovkin, I.V. Bordenjuk. **Scattering of conduction electrons on the W(001) surface covered with deuterium monolayer: the role of surface electronic states** (*Institute of Physics, NAS of Ukraine, Kyiv*).
8. **L.S. Andriyko**, O.V. Goncharuk, V.M. Gun'ko. **Effects of ions on the properties of aqueous suspensions of nanosilica** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
9. **D.Yu. Balakin**, L.Yu. Lopandya, D.V. Stryzhus. **Formation of BeO on molybdenum (110) surface** (*Institute of Physics, NAS of Ukraine, Kyiv*).
10. **V. Halysh**[1,2], I. Deykun[1], I. Trembus[1]. **Influence of delignification conditions of solid agricultural wastes on the composition of spent solutions** ([1]*Department of Ecology and Plant Polymers Technology, National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute",* [2]*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
11. **O.I. Gichan**. **Understanding the concentration distribution in the near-electrode layer in the course of a homogeneous chemical reaction of first order under a model electrocatalytic process** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
12. **Yu.A. Kamysh**, I.V. Shapochkina. **The theory of photomotors: stochastic processes with deterministically changing transition rates** (*Belarusian State University, Minsk*).

13. **A. Karelina**[1], V. Sliesarenko[2], O. Dudarko[2], O. Solcova[3]. **Sorption of dichromate anions on mesoporous silica, functionalized with aminopropyl groups** (*[1]National University of "Kyiv-Mohyla Academy", Ukraine, [2]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv, [3]Institute of Chemical Process Fundamentals of the ASCR, v.v.i., Prague, Czech Republic*).
14. **O.D. Kochkodan**, N.M. Antraptseva, V.I. Maksin, R.S. Zhila. **Adsorption of surfactants mixtures from aqueous solutions by carbon sorbents** (*National University of Life and Environmental Sciences of Ukraine, Kyiv*).
15. **T.Ye. Korochkova**[1], I.V. Shapochkina[2], V.M. Rozenbaum[1]. **Symmetry properties of Brownian motors with fluctuating periodic potential energy** (*[1]Chuiko Institute of Surface Chemistry of NAS of Ukraine, Kyiv, [2]Department of Physics, Belarusian State University, Minsk*).
16. **T.Ye. Кorochkova**. **Piecewise-linear approximation of the potential relief of a Brownian motors** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
17. **L.M. Lugina**[1], N.G. Kobylinska[2]. O.A. Dudarko[3]. **Removal of trace amount of dyes from aqueous solution by polyfunctional N-, P-, S-containing silica** (*[1]National University of Kyiv-Mohyla Academy, [2]Faculty of Chemistry, Taras Shevchenko National University of Kyiv, Ukraine, [3]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
18. **F.D. Manilevich**, A.V. Kutsyi. **Tungsten carbide based cathodes modified with titanium or hafnium for hydrogen evolution from water** (*Vernadsky Institute of General & Inorganic Chemistry, NAS of Ukraine, Kyiv*).
19. **I.P. Olyshevets**[1], O.V. Severinovskaya[2], V.A. Ovchynnikov[1], V.M. Amirkhanov[1]. **Synthesis and mass spectrometric investigation of lanthanide complexes with polydentate carbacylamidophosphates (CAPh ligands)** (*[1]Taras Shevchenko National University of Kyiv, Ukraine, [2]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
20. **N. Osipova**, T. Kvernadze, N. Burkiashvili. **Georgian natural zeolites for treatment of sewage waters** (*Petre Melikishvili Institute of Physical and Organic Chemistry, Ivane Javakhishvili Tbilisi State University, Georgia*).
21. **N.V. Roik**, L.A. Belyakova, M.O. Dziazko. **pH-Sensing properties of transparent silica film with chemically immobilized alizarin yellow** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
22. **M. Sęczkowska**[1], M.V. Galaburda[2], V.M. Bogatyrov[2], A. Deryło-Marczewska[1], A.W. Marczewski[1], A. Chrzanowska[1]. **Preparation and comparison of structural and adsorption properties of active carbons obtained from nutshells** (*[1]Faculty of Chemistry, Maria Curie-Sklodowska University, Lublin, Poland, [2]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
23. A. Chrzanowska, A. Deryło-Marczewska, **M. Sęczkowska**. **Biopolymer/porous silica support: spectroscopic characteristics of biocomposite surface** (*Faculty of Chemistry, Maria Curie-Sklodowska University, Lublin, Poland*).
24. T.M. Budnyak[1,2], S. Aminzadeh[3], Ie.V. Pylypchuk[2], V.A. Tertykh[2], M.E. Lindström[1], **O. Sevastyanova**[1,3]. **Functional lignin-silica hybrids for water purification: peculiarities of synthesis and application** (*[1]Department of Fiber and Polymer Technology, KTH Royal Institute of Technology, Stockholm, Sweden, [2]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv, [3]Wallenberg Wood Science Center (WWSC), Department of Fiber and Polymer Technology, KTH Royal Institute of Technology, Stockholm, Sweden*).

25. **O.V. Severinovskaya**[1], Y.M. Dovbii[2], V.Y. Chernii[2], I.M. Tretyakova[2], A.V. Gorski[3]. **MALDI and GALDI mass spectrometry investigation of fragmentation of zirconium and hafnium phthalocyanines with out-of-plane ligands** ([1]*Chuiko Institute of Surface Chemistry, NAS of Ukraine,* [2]*Vernadsky Institute of General and Inorganic Chemistry, NAS of Ukraine, Kyiv,* [3]*Institute of Physical Chemistry Polish Academy of Sciences, Warsaw*).
26. V.M. Rozenbaum[1], **I.V. Shapochkina**[2], Y. Teranishi[3], L.I. Trakhtenberg[4]. **Fluctuations of different nature in the theory of high-temperature ratchets** ([1]*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv,* [2]*Belarusian State University, Minsk,* [3]*Institute of Physics, National Chiao Tung University, Hsinchu, Taiwan,* [4]*Semenov Institute of Chemical Physics, RAS, Moscow*).
27. V.M. Rozenbaum[1], **I.V. Shapochkina**[2], Y. Teranishi[3], L.I. Trakhtenberg[4]. **Hidden symmetries of pulsating ratchets** ([1]*Chuiko Institute of Surface Chemistry of NAS of Ukraine, Kyiv,* [2]*Belarusian State University, Minsk,* [3]*Institute of Physics, National Chiao Tung University, Hsinchu, Taiwan,* [4]*Semenov Institute of Chemical Physics, RAS, Moscow*).
28. **A.A. Shapoval**, E.M. Panov, I.O. Shapoval. **Physical processes and crisis modes when boiling water on porous metal surfaces** (*National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute"*).
29. **E.A. Streltsova**, A.A. Mazuryk. **Synergism and antagonism of the action of non-ionic and cationic surfactants during their mutual adsorption on paraffin** (*Faculty of Chemistry, Odessa I.I. Mechnikov National University, Ukraine*).
30. **I.Ya. Sulym**[1], P. Veteška[2], A. Gatial[2], R. Klement[3], M.V. Borysenko[1], M. Janek[2,4]. **Spectroscopic and optical properties of erbium and ytterbium doped transparent silica glasses prepared by sol –gel process** ([1]*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv,* [2]*Faculty of Chemical and Food Technology, Slovak University of Technology, Bratislava,* [3]*FunGlass - Centre for Functional and Surface Functionalized Glass, Trenčín,* [4]*Faculty of Natural Sciences, Comenius University, Bratislava, Slovak Republic*).
31. **V.G. Tsitsishvili**, N.M. Dolaberidze, M.O. Nijaradze, N.A. Mirdzveli. **Preparation of SOD type zeolite from perlite** (*Petre Melikishvili Institute of Physical and Organic Chemistry, Ivane Javakhishvili Tbilisi State University, Georgia*).
32. **A.F. Tymchuk**. **Surfactants and natural polymers in flocculation process** (*Odessa I.I. Mechnikov National University, Ukraine*).
33. **A.A. Zhokh**, P.E. Strizhak. **Non-Fickian diffusion in mesoporous media: adsorption induced** (*L.V. Pisarzhevskii Institute of Physical Chemistry, NAS of Ukraine, Kyiv*).
34. **A.Yu. Zhuravlov**, A.V. Shijan, N.A. Semenov, B.M. Shirokov. **Gas-phase deposition of a cavitation-resistant coating based on boron carbide** (*National Science Center "Kharkov Institute of Physics and Technology", Ukraine*).
35. **U.A. Vysotskaya**, I.V. Shapochkina. **Some features of high-temperature Brownian ratchets governing by small harmonic fluctuations of potential energy** (*Belarusian State University, Minsk*).

3. Chemistry, Physics and Technology of Nanomaterials

36. P.P. Gorbyk, I.V. Dubrovin, **N.V. Abramov**. **Synthesis and magnetic properties of nanocrystals of solid solutions** $(Y_{1-x}La_x)_3Fe_5O_{12}$ (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).

37. **L.A. Andryushchenko**[1], A.M. Kudin[1], A.L. Shpilinskaya[2], A.V. Didenko[2]. **The method of applying a protective hydrophobic coating on the surface of CsI scintillator** (*[1]National University of Civil Protection of Ukraine, [2]Institute for Scintillation Materials, NAS of Ukraine, Kharkov*).
38. **T.S. Antonenko**, N.O. Dudchenko, A.B. Brik. **Transformation of the magnetic properties of synthetic goethite and hematite in an aqueous medium** (*M.P. Semenenko Institute of Geochemistry, Mineralogy and Ore Formation, NAS of Ukraine, Kyiv*).
39. T.Y. Shermatov, **R.Kh. Ashurov**. **Size-controlled synthesis of nanocrystalline silicon dioxide by Stöber process** (*Institute of Ion Plasma & Laser Technologies, NAS of Uzbekistan, Tashkent*).
40. **F. Azimov**, O. Sanzhak, D. Brazhnyk. **Influence of nitrogen implanted in titania-stainless steel on photocatalytic activity** (*Institute for Sorption and Problems of Endoecology, NAS of Ukraine, Kyiv*).
41. **O.V. Bespalko**[1,2], N.V. Stolyarchuk[2], V.V. Tomina[2], M. Vaclavikova[3], I.V. Melnyk[2,3]. **The formation of polysilsesquioxane-based materials with bifunctional surface layer** (*[1]National University of "Kyiv-Mohyla Academy", Ukraine, [2]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv, [3]Institute of Geotechnics SAS, Kosice, Slovak Republic*).
42. **Yu. Bolbukh**, R. Kozakevych, V. Tertykh. **Polymeric composites for biocompatible coatings** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
43. **M. Bondarenko**, P. Silenko, N. Gubareni, O. Khyzhun, N. Ostapovskaya. **Synthesis carbon nitride films onto Ti substrate by thermal CVD melamine** (*Frantsevich Institute for Problems of Materials Science, NAS of Ukraine, Kyiv*).
44. **M. Bondarenko**[1], T. Khalyavka[1], S. Camyshan[1], I. Petrik[2], N. Shcherban[3], N. Tsyba[1]. **Photocatalytic properties of S/TiO_2 nanocomposites** (*[1]Institute for Sorption and Problems of Endoecology, NAS of Ukraine, [2]Chuiko Institute of Surface Chemistry, NAS of Ukraine, [3]L.V. Pisarzhevskii Institute of Physical Chemistry, NAS of Ukraine, Kyiv*).
45. **Yu.O. Budash**, N.M. Rezanova, V.P. Plavan. **Structure and properties of nanofilled microfibrillary threads** (*Kyiv National University of Technologies and Design, Ukraine*).
46. **O.A. Cherniuk**, S.V. Zhuravsky, Yu.I. Sementsov, M.T. Kartel. **The pyrogenic synthesis of a complex metal-oxide catalyst for the growth of carbon nanotubes** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
47. V.M. Rozenbaum[1], **M.L. Dekhtyar**[2], L.I. Trakhtenberg[3]. **Effect of electron transition kinetics on the photomotor velocity** (*[1]Chuiko Institute of Surface Chemistry, NAS of Ukraine, [2]Institute of Organic Chemistry, NAS of Ukraine, Kyiv, [3]Semenov Institute of Chemical Physics, RAS, Moscow*).
48. **D.V. Doroshenko**, I.V. Pylypenko, B.Yu. Kornilovych. **Semi-synthetic adsorbents based on montmorillonite and silica gel** (*Department of Chemical Technology of Ceramics and Glass, Faculty of Chemical Technology, National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute"*).
49. **Yu.S. Dzyazko**[1], V.M. Ogenko[1], A.V. Palchik[1], T.V. Maltseva[1], Yu.M. Volfkovich[2], V.E. Sosenkin[2]. **Nanocomposites based on inorganic ion exchangers and carbon materials** (*[1]Vernadsky Institute of General and Inorganic Chemistry, NAS of Ukraine, Kyiv, [2]A.N. Frumkin Institute of Physical Chemistry and Electrochemistry, Moscow, RF*).
50. **P.V. Galiy**[1], T.M. Nenchuk[1], I.R. Yarovets'[1], I.O. Poplavskyy[2], Ya.M. Buzhuk[1]. **Formation of sub- and monolayer nanosystems metal-layered semiconductor** (*[1]Ivan Franko Lviv National University, Ukraine, [2]Vasyl Stefanyk Precarpatian National University, Ivano-Frankivsk, Ukraine*).
51. **O.V. Goncharuk**[1], O.I. Shipul[2], O.V. Ishchenko[2], A.G. Dyachenko[2], E.M. Pakhlov[1], M.V. Borysenko[1], Yu.I. Gornikov[1], O.I. Oranska[1]. **Synthesis and investigation of**

structural features of silica-supported nanocomposites with nickel and cobalt oxides (*[1]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv, [2]Faculty of Chemistry, Taras Shevchenko National University of Kyiv, Ukraine*).

52. **M.N. Goroneskul**, L.A. Andryushchenko, A.M. Kudin. **Nanocomposite coatings for protective firefighter uniforms with improved performance characteristics** (*National University of Civil Protection of Ukraine, Kharkov*).
53. **A.M. Grinko**[1], A.V. Brichka[2], O.M. Bakalinska[2], S.Ya. Brichka[2], M.T. Kartel[2]. **Preparation, characterization and catalytic activity of nanoceria** (*[1]National University of "Kyiv-Mohyla Academy", Ukraine, [2]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
54. **N.V. Guzenko**[1], P. Lodewyckx[2], K. László[3], M. Thommes[4]. **Effect of structure and chemical state of activated carbon surface on water adsorption** (*[1]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv, [2]Royal Military Academy, Department of Chemistry, Brussels, Belgium, [3]Budapest University of Technology and Economics, Hungary, [4]Quantachrome Instruments, Boynton Beach, USA*).
55. **O.O. Havryliuk**, O.Yu. Semchuk. **Interaction of visible electromagnetic radiation with periodic nanostructures** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
56. L.V. Karabanova, **L.A. Honcharova**, N.V. Babkina. **Sorption and mechanical properties of POSS-containing nanocomposites based on PU/PHPMA semi-IPNs** (*Institute of Macromolecular Chemistry, NAS of Ukraine, Kyiv*).
57. **D. Ihnatiuk**, O. Linnik. **Monitoring of structural and surface properties of platinum ions doped titania films with different surface morphology** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
58. **G. Ilnitska**[1], M. Marinich[1], N. Oliinyk[1], G. Bazaliy[1], I. Zaitseva[1], H. Ishchenko[2], S. Gaidai[2]. **Effect of physicochemical actions on surface properties of diamond nanopowders** (*[1]N. Bakul Institute for Superhard Materials, NAS of Ukraine, Kyiv, [2]Taras Shevchenko National University of Kyiv, Ukraine*).
59. V.A. Bogatyrenko[1], **I.V. Kalinin**[1], M.M. Tsiba[2]. **Synthesis and properties of nano-structured silica, modified by nitrogen-containing compounds** (*[1]National Pedagogical Dragomanov University, Kyiv, Ukraine, [2]Institute for Sorption and Problems of Endoecology, NAS of Ukraine, Kyiv*).
60. **L.S. Kaykan**[1], J.S. Mazurenko[2], V.S. Bushkova[2], A.I. Kachmar[2]. **Effect of substitution of magnesium ions on the structure and morphology of nanoscale lithium ferrite** (*[1]G.V. Kurdyumov Institute for Metal Physics, NAS of Ukraine, Kyiv, [2]Vasyl Stefanyk Precarpathian National University, Ivano-Frankivsk, Ukraine*).
61. **N.I. Khripta**, B.N. Mordyuk, O.P. Karasevska. **Effects of ultrasonic impact treatment on physical and chemical state of the surface layer of Zr1Nb alloy** (*G.V. Kurdyumov Institute for Metal Physics, NAS of Ukraine, Kyiv*).
62. **L.M. Kokhtych**, V.R. Lyakhovetskiy, T.N. Smirnova. **Nonlinear diffraction of volume structures based on metal nanoparticles** (*Institute of Physics, NAS of Ukraine, Kyiv*).
63. **I.S. Kolesnyk**, O.O. Kravchenko, V.V. Konovalova, A.F. Burban. **Polyvinylidene fluoride membranes modification with TiO_2 nanoparticles** (*National University of "Kyiv-Mohyla Academy", Ukraine*).
64. **D.M. Korytko**, S.A. Alekseev. **Nanoscale anodization products of silicon carbide** (*Faculty of Chemistry, Taras Shevchenko National University of Kyiv, Ukraine*).
65. **T. Kulik**[1], A. Varga[2], B. Palianytsia[1], O. Naumov[2], M. Wagner[2], B. Abel[2]. **Study of the thermal stability of nitrogen-containing graphene by using TPD-MS** (*[1]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv, [2]Chemical Department, Leibniz Institute of Surface Modification, Leipzig, Germany*).

66. **T. Kulik**[1], N. Nastasienko[1], B. Palianytsia[1], M. Larsson[2], M. Kartel[1]. **Thermal transformation of cinnamic and aliphatic carboxylic acids on the nanoceria surface** (*[1]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv, [2]Stockholm University, AlbaNova University Center, Department of Physics, Sweden*).
67. **M.M. Kurmach**, K.M. Konysheva, P.S. Yaremov, O.V. Shvets. **Hierarchical zeolites with BEA, MFI, MTW and MOR topology overgrown on expanded obsidian or perlite** (*L.V. Pisarzhevskii Institute of Physical Chemistry, NAS of Ukraine, Kyiv*).
68. **P.O. Kuzema**, Yu.M. Bolbukh, V.A. Tertykh. **Luminescent materials based on organic salts pyrolyzed at the silica surface** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
69. B.S. Kolupaev, **V.V. Levchuk**. **The relationship between the physical and chemical properties of polymer nanodisperse systems** (*Rivne State University of Humanities, Ukraine*).
70. **O.M. Lisova**, S.M. Makhno, G.M. Gunya, P.P. Gorbyk. **Electrophysical properties of carbon nanotubes / NiCo composites** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
71. **B.V. Lopushanska**[1], Yu.M. Azhniuk[1,2], V.V. Lopushansky[2], V.M. Dzhagan[3], I.P. Studenyak[1], A.V. Gomonnai[1,2], A.E. Rayevskaya[4,5], O.L. Stroyuk[4,5]. **Optical studies of CdSe nanocrystals grown from aqueous solutions in the presence of gelatin** (*[1]Uzhhorod National University, Ukraine, [2]Institute of Electron Physics, NAS of Ukraine, Uzhhorod, [3]V. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine, [4]L.V. Pysarzhevskii Institute of Physical Chemistry, NAS of Ukraine, Kyiv, [5]Technische Universität Dresden, Germany*).
72. **O. Lorenz**, K. Hanus, A. Varga. **Long-term stability of sodium oxygen batteries** (*Leibniz Institute of Surface Engineering (IOM), Leipzig, Germany*).
73. **D.Yu. Lyashenko**, L.A. Belyakova. **Interaction of β-cyclodextrin with 2,4-dihydroxybenzoic acid in aqueous solutions** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
74. **O.Yu. Makido**, G.I. Khovanets’, O.Yu. Khavunko. **Organometallic composites with catalytic properties based on TEOS and transition metal salts** (*Department of Physical Chemistry of Fossil Fuels of the Institute of Physical–Organic Chemistry and Coal Chemistry named after L.M. Lytvynenko, NAS of Ukraine, Lviv*).
75. B.B. Kolupaev[1], **Yu.R. Maksymtsev**[2]. **Physical-chemical technologies for the production of metal-dispersed polymer systems** (*[1]Institute of Cybernetics of the Rivne International Economic and Humanitarian University named after Academician S. Demyanchuk, Rivne, [2]Rivne State University of Humanities, Ukraine*).
76. S.L. Prokopenko, **R.V. Mazurenko**, O.I. Oranska, G.M. Gunya, S.N. Makhno, P.P. Gorbyk. **Electrophysical characteristics of polymer nanocomposites based on carbon nanotubes/ferrites modified copper iodide** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
77. **I.V. Melnyk**[1,2], M. Vaclavikova[2]. **Selective removal of precious metals by materials with ethylthiocarbamidepropyl groups** (*[1]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv, [2]Institute of Geotechnics, Slovak Academy of Sciences, Kosice*).
78. **B.M. Mordyuk**, S.Yu. Makarenko, A.V. Proshak, P.Yu. Volosevich, V.Ye. Panarin, M.Ye. Svavilny, M.A. Skoryk. **Corrosion behaviour of high-entropy AlCuCrCoNiFe nanostructured coatings obtained by physical vapour deposition method with cathode arc evaporation (PVD CAE)** (*G.V. Kurdyumov Institute for Metal Physics, NAS of Ukraine, Kyiv*).

79. **O.V. Mykhailenko**[1], A.V. Strungar[2], Yu.I. Prylutskyy[1], I.V. Komarov[1], O.O. Mykhailenko[1], O.Yu. Lagerna[1]. **Complexing of fullerene C_{60} with some metal lactates: quantum chemical simulation** (*[1]Taras Shevchenko National University of Kyiv, Ukraine, [2]Vernadsky National Library of Ukraine, Kyiv*).
80. **L.V. Nosach**[1], E.F. Voronin[1], P. Klonos[2], A. Kyritsis[2], P. Pissis[2], J. Skubiszewska-Zięba[3], H. Waniak-Nowicka[3]. **Morphology of SiO_2/PDMS nanocomposites** (*[1]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv, [2]Department of Physics, National Technical University of Athens, Greece, [3]Faculty of Chemistry, Maria Curie-Skłodowska University, Lublin, Poland*).
81. **V.M. Ogenko**, O.M. Korduban, T.V. Kryshchuk. **Investigation of nitrogen-modified graphene by the XPS method** (*Vernadsky Institute of General & Inorganic Chemistry, NAS Ukraine, Kyiv*).
82. **M.I. Pas'ko**[1], A.M. Prudnikov[2], R.V. Shalaev[2]. **Structure and magnetic properties of Ni-C hybrid nanofilms** (*[1]Donetsk National Medical University, Lyman, Ukraine, [2]Donetsk Institute for Physics and Engineering, NAS of Ukraine, Kyiv*).
83. **M.V. Pasichnyk**. **Network characteristic of films with styrene-acrylic polymer and dispersion of silver nanoparticles** (*Mykolaiv National University named after V.O. Sukhomlynsky, Department of Chemistry and Biochemistry, Ukraine*).
84. **E.N. Poddenezhny**[1], O.V. Davydova[1], N.E. Drobyshevskaya[1], A.A. Boiko[1], M.V. Borysenko[2]. **Green phosphor Y_2O_3 Tb^{3+} nanostructured powders prepared by the combustion method** (*[1]Sukhoi Gomel State Technical University, Belarus, [2]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
85. **S.L. Prokopenko**, R.V. Mazurenko, O.I. Oranska, G.M. Gunya, S.N. Makhno, P.P. Gorbyk. **Electrophysical characteristics of polymer nanocomposites based on barium hexaferrite modified copper iodide** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
86. **O.V. Protsenko**[1], O.A. Dudka[1], Y.S. Yasinskiy[1], M.N. Borovaya[2], A.P. Naumenko[3], I.I. Horiunova[2], S.H. Plohovska[2], A.S. Postovoytova[2], Ya.V. Pirko[2], A.I. Yemets[2], S.V. Demidov[1], I.A. Kozeretska[1]. **Biological synthesis of Ag_2S nanoparticles and study their antibacterial properties** (*[1]Taras Shevchenko National University of Kyiv, [2]Institute of Food Biotechnology and Genomics, NAS of Ukraine, Kyiv, [3]Faculty of Physics, Taras Shevchenko National University of Kyiv, Ukraine*).
87. **O.I. Shkromada**[1], O.G. Bordunova[1], A.G. Ryabishev[2], E.A. Mironets[2], A.A. Stepanenko[3], V.D. Chivanov[2], A.V. Kochenko[2], E.I. Zinchenko[2]. **Thermal decomposition behaviour of plastering and cement building materials modified by biocides composition for veterinary medicine** (*[1]Sumy National Agrarian University, [2]Institute of Applied Physics, NAS of Ukraine, Sumy, [3]Sumy State University, Ukraine*).
88. **A.I. Senenko**[1], V.V. Cherepanov[1], O.A. Marchenko[1], Yu.I. Prylutskyy[1,2], A.G. Naumovets[1]. **AFM and STM investigations of nanoparticles used to improve chemotherapy effectiveness** (*[1]Institute of Physics, NAS of Ukraine, Kyiv, [2]Taras Shevchenko National University of Kyiv, Ukraine*).
89. B.B. Kolupaev[1], **V.O. Sidletskyi**[2]. **Components of the energy spectrum of the interaction of a polymer-nanodispersed metal** (*[1]Institute of Cybernetics of the Rivne International Economic and Humanitarian University named after Academician S. Demyanchuk, Rivne, [2]Rivne State University of Humanities, Ukraine*).
90. **N.V. Sigareva**[1], I.M. Mykytyn[2], I.F. Myroniuk[2], N.V. Abramov[1], B.M. Gorelov[1], V.M. Mishchenko[1], D.L. Starokadomsky[1]. **Magnetic and mechanical properties of epoxy magnetocomposites** (*[1]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv, [2]Vasyl Stefanyk Precarpathian National University, Ivano-Frankivsk, Ukraine*).

91. **O.G. Sirenko**, S.M. Makhno, O.M. Lisova, G.M. Gunya, P.P. Gorbyk. **Electrophysical properties of composites based on the epoxy resin and thermally expended graphite** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
92. **N. Smirnova**[1], I. Petrik[1], O. Linnik[1], A. Eremenko[1], V. Vorobets[2], G. Kolbasov[2]. **Photo- and electrocatalytic activity of TiO_2 based films: effect of metal ion's doping** (*[1]Chuiko Institute of Surface Chemistry, NAS of Ukraine, [2]Vernadsky Institute of General & Inorganic Chemistry, NAS of Ukraine, Kyiv*).
93. **H.M. Starukh. The peculiarities of CuI formation on the surface of ZnAl layered double hydroxides** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
94. **M. Studziński**[1], Y.M. Bolbukh[2], I. Malinowska[1], V.A. Tertykh[2]. **Magnetite-silica materials with modified surface, synthesis and sorption abilities of organic compounds** (*[1]Planar Chromatography Department, Chair of Physical Chemistry, Faculty of Chemistry, Maria Curie-Skłodowska University, Lublin, Poland, [2]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
95. **E. Trusova**[1], Y. Tratsiak[2], M. Korjik[3]. **Silicates glass and glass-ceramics activated RRE-ions are promising materials for scintillation and luminescence's applications** (*[1]Belarusian State Technological University, [2]Research Institute for Physical Chemical Problems Belarusian State University, [3]Institute for Nuclear Problems, Belarus State University, Minsk).*
96. **V.V. Tytarenko**, V.A. Zabludovsky, E.Ph. Shtapenko. **Mechanical and protective properties of composite nickel coatings** (*Dnepropetrovsk National University of Railway Transport named after academician V. Lazaryan, Dnipro, Ukraine*).
97. **N.V. Zhdanyuk**[1], V.Yu. Tobilko[1], I.A. Kovalchuk[2]. **Sorption of U (VI) ions by montmorillonite and organomontmorillonite modified by nanosized zero-valent iron** (*[1]National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", Ukraine, [2]Institute for Sorption and Problems of Endoecology, NAS of Ukraine, Kyiv*).
98. **M.M. Zhyhailo**, O.I. Demchyna, Kh.V. Rymsha, I.Yu. Yevchuk. **Organic-inorganic nanocomposites based on acrylates and 3-methacryloxypropyltrimethoxysilane** (*Department of Physico-chemistry of Fossil Fuels L.M. Lytvynenko Institute of Physico-organic Chemistry and Coal Chemistry, NAS of Ukraine, Lviv*).

4. Medical, Biological and Biochemical Aspects of Studies of Highly Disperse Materials

99. **A.N. Bagatskaya**, R.V. Mazurenko, S.N. Makhno, P.P. Gorbyk. **The effect of carbon nanotubes on the enzymatic activity of the yeast cells *Saccharomyces cerevisiae*** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
100. **V.M. Bogatyrov**[1], M.V. Galaburda[1], V.M. Gun'ko[1], T.V. Rudenchyk[2], R.A. Rozhnova[2], N.A. Galatenko[2], K.S. Tsyganenko[3], Ya.I. Savchuk[3], M.S. Kharchuk[3] **Antibacterial silica fillers and polymer composites for medical applications** (*[1]Chuiko Institute of Surface Chemistry, NAS of Ukraine, [2]Institute of Macromolecular Chemistry, NAS of Ukraine, [3]Zabolotny Institute of Microbiology and Virology, NAS of Ukraine, Kyiv*).
101. **O.G. Bordunova**[1], E.G. Astrakhantseva[1], R.V. Denisov[1], O.O. Chekh[1], A.G. Ryabishev[2], E.A. Mironets[2], A.A. Stepanenko[3], V.D. Chivanov[2], A.V. Kochenko[2], E.I. Zinchenko[2]. **Analysis for thermal decomposition of calcite biocrystalline structures from bird's hatching and food eggs** (*[1]Sumy National Agrarian University, [2]Institute of Applied Physics, NAS of Ukraine, Sumy, [3]Sumy State University, Ukraine*).

102. **T.V. Cherniavska**[1], M.A. Boretska[2], A.A. Protasov[3], I.A. Morozovskaya[3], O.P. Tarasyuk[4], O.V. Dzhuzha[4], S.P. Rogalsky[4]. **New antifouling paint containing polymeric biocide polyhexamethylene guanidine molybdate** ([1]*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv,* [2]*University Duisburg-Essen, Biofilm Centre, Germany,* [3]*Institute of Hydrobiology, NAS of Ukraine,* [4]*Institute of Bioorganic Chemistry and Petrochemistry, NAS of Ukraine, Kyiv*).
103. **V.D. Chivanov**[1], O.G. Bordunova[2], A.G. Ryabishev[1], A.N. Kalinkevich[1], E.A. Mironets[1], A.A. Stepanenko[3], A.V. Kochenko[1], E.I. Zinchenko[1], S.N. Danilchenko[1]. **Correlating structural changes and gas evolution during the thermal decomposition of mollusc shell** ([1]*Institute of Applied Physics, NAS of Ukraine, Sumy,* [2]*Sumy National Agrarian University,* [3]*Sumy State University, Ukraine*).
104. **E. Dikhtiaruk**[1], V. Gun`ko[2], V. Paientko[2], A. Matkovsky[2], S. Alekseev[1], Yu. Gornikov[2]. **Synthesis and properties of cryogels for medical applications** ([1]*Taras Shevchenko National University of Kyiv, Ukraine,* [2]*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
105. **A.P. Golovan**[1], T.V. Krupska[1], T. Lupaşcu[2], O. Spinu[2], V.V. Turov[1]. **Effect of nanosilica-Enoxil composite systems on morphological parameters sprouts tomatoes** ([1]*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv,* [2]*Institute of Chemistry of the ASM, Chişinău, Moldavia*).
106. V.V. Strelko, V.F. Lapko, **E.V. Isaieva**, M.F. Kovtun, V.V. Berezhnaya. **Ion-exchange and bactericidal properties of oxidized carbons with adsorbed ions of silver, copper and zinc** (*Institute for Sorption and Problems of Endoecology, NAS of Ukraine, Kyiv*).
107. **I.A. Farbun**, Y.V. Isaieva, V.A. Trychlib, N.N. Tsyba. **Adsorption of physiologically active substances by medical carbon adsorbents with different bulk density** (*Institute for Sorption and Problems of Endoecology, NAS of Ukraine, Kyiv*).
108. **O.O. Kazakova**, N.N. Vlasova, L.P. Golovkova. **Effect of bile salts on adsorption of cholesterol on hydrophilic/hydrophobic silica surface** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
109. **N.Y. Klymenko**, I.V. Siora, E.A. Novikova, A.P. Golovan, T.V. Krupska, V.V. Turov. **Destruction of hydrocarbons by composite system based on the nanosilicas and yeast cells mixture in aqueous medium** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
110. **N.O. Lipkovska**[1], V.M. Barvinchenko[1], T.V. Kulik[1], M. Larsson[2], M.T. Kartel[1]. **Adsorption of natural cinnamic acids on the nanoceria surface** ([1]*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv,* [2]*Stockholm University, AlbaNova University Center, Department of Physics, Sweden*).
111. **O.V. Markitan**, N.N. Vlasova. **Pyrimidine nucleotide complexes on the nanocrystalline titania surface** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
112. **T. Mykhailova**[1], V. Konovalova[1], A. Marinin[2]. **Synthesis of chitosan microemulsions by membrane emulsification** ([1]*National University of "Kyiv-Mohyla Academy", Ukraine,* [2]*National University of Food Technologies, Kyiv, Ukraine*).
113. **O.M. Nesterenko**[1,3], T.S. Gergelyuk[1,3], O.M. Perepelytsina[1], M.V. Sidorenko[1], O.M. Bakalinska[2], L.I. Ostapchenko[3]. **Efficiency of binding of doxorubicin to CNTs and its release during incubation with trypsin** ([1]*Department for Biotechnical Problems of Diagnostic, Institute for Problems of Cryobiology and Cryomedicine, NAS of Ukraine,* [2]*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv,* [3]*Educational and Scientific Centre "Institute of Biology and Medicine", Taras Shevchenko National University of Kyiv, Ukraine*).

114. **N.M. Opanashchuk**[1], A.P. Kusyak[2], A.L. Petranovska[1], P.P. Gordyk[1]. **Magnetically sensitive nanocomposites for targeted transport of Gemcitabine anticancer drug** ([1]*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv,* [2]*Zhytomyr State University named after Ivan Franko, Ukraine*).
115. **V.V. Paientko**[1], A.K. Matkovsky[1], O.I. Oranska[1], Yu.I. Gornikov[1], Yu.M. Nichiporuk[1], A.V. Korobeinyk[1], O.S. Kisenko[2]. **Physicochemical properties of clay adsorbents for oral administration** ([1]*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv,* [2]*Sole entrepreneur Viktor Krasavin, Ukraine*).
116. **A.V. Pavlenok**[1], O.V. Davydova[1], E.N. Poddenezhny[1], N.E. Drobyshevskaya[1], A.A. Boiko[1], M.V. Borysenko[2]. **Preparation and properties of biodegradable composite materials based on polyvinyl alcohol and starch** ([1]*Sukhoi Gomel State Technical University, Belarus,* [2]*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
117. **V. Porubleva**[1], N. Vityuk[1], Iu. Mukha[1], N. Smirnova[1], R. Linnik[2], M. Malysheva[2]. **Spectroscopic study of products of photoinduced reaction between gold and tryptophan** ([1]*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv,* [2]*Department of Chemistry, Taras Shevchenko National University of Kyiv, Ukraine*).
118. **A.O. Rugal**, T.V. Krupska, V.V. Turov. **Silica-based laevomycetin controlled release nanocomposite** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
119. **I.O. Skorochod**, I.K. Kurdish. **Influence of bentonite nanoparticles and nano-SiO_2 on the total content of the phenolic compounds in the cultural medium of bacteria *Azotobacter vinelandii* IMV B-7076** (*Zabolotny Institute of Microbiology and Virology, NAS of Ukraine, Kyiv*).
120. **O. Skurikhina**[1], R. Kozakevych[2], A. Omelchuk[1], O. Liubatska[1], T. Murlanova[1], P. Vakuliuk[1], A. Golub[1], V. Tertykh[2]. **Investigation of Ornidazole desorption from the nanocomposites based on silica** ([1]*National University of "Kyiv-Mohyla Acsdemy", Ukraine,* [2]*Chuiko Institute of Surface Chemistry of the NAS of Ukraine, Kyiv).*
121. **L.P. Storozhuk**, A.L. Petranovska, P.P. Gorbyk. **Magnetic fluid with high dispersion for hyperthermia purpose** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
122. **N.B. Zhorzholiani**, L.A. Metreveli, K.D. Amirkhanashvili, V.G. Tsitsishvili, O.G. Lomtadze. **Tetra-acid complexes of trimecaine** (*Petre Melikishvili Institute of Physical and Organic Chemistry; Ivane Javakhishvili Tbilisi State University, Georgia).*
123. **N. Uludag**. **Synthesis route to the strychnos-type alkaloids** (*Faculty of Science and Arts, Department of Chemistry, Namık Kemal University, Tekirdag, Turkey*).
124. **N. Uludag**. **A new route to the deethylaspidospermidine** (*Faculty of Science and Arts, Department of Chemistry, Namık Kemal University, Tekirdag, Turkey*).
125. **N.V. Yelahina**[1], T.V. Krupskaya[1], P. Jovaišas[2], R. Bieliauskienė[2], B. Charmas[3], V.V. Turov[1]. **Hydrated properties of the composite system based on high-dispersed silica and *Amanita muscaria*** ([1]*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv,* [2]*"Silicio Biotechnologijos" PJSC, Vilnius, Lithuania,* [3]*Maria Curie-Sklodowska University, Lublin, Poland*).
126. **N. Vityuk**[1], Iu. Mukha[1], N. Andriushyna[2,3]. **The effect of Pluronic on gold nanoparticles synthesized in the presence of tryptophan** ([1]*Chuiko Institute of Surface Chemistry, NAS of Ukraine,* [2]*L.V. Pisarzhevskii Institute of Physical Chemistry, NAS of Ukraine,* [3]*NanoMedTech LLC, Kyiv, Ukraine*).
127. **E.F. Voronin**, L.P. Golovkova, E.M. Pakhlov, L.V. Nosach. **Effect of mechanical and ultrasonic treatment of nanosilica aqueous suspension on gelatin adsorption** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).

Synthesis and magnetic properties of nanocrystals of solid solutions $(Y_{1-x}La_x)_3Fe_5O_{12}$

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Different magnetic dosage forms: ointments, magnetic suppositories, patches, *etc*. currently are widely used in medicine. Their therapeutic and diagnostic effectiveness has been proven by many researchers. Therapeutic action of magnetic drugs is due to the presence of magnetic filler. Quantitative content of magnetic filler and its quality determine the therapeutic properties of magnetic dosage forms.

Nano-sized particles of magnetite and ferrites of transition metals due to their high magnetization and low toxicity are used for targeted drug delivery, in the method of magnetic hyperthermia, in magnetic resonance imaging and for diagnosis of diseases. The size of the particles should be 10 - 20 nm, that is, they should be superparamagnetic (residual magnetization should be zero) at room temperature and normal (37 °C) temperature. The range of substances and methods of synthesis of the above-mentioned materials is constantly expanding. Yttrium iron garnet $Y_3Fe_5O_{12}$, lantan iron garnet $La_3Fe_5O_{12}$ and single-domain nanoparticles of their solid solutions were synthesized.

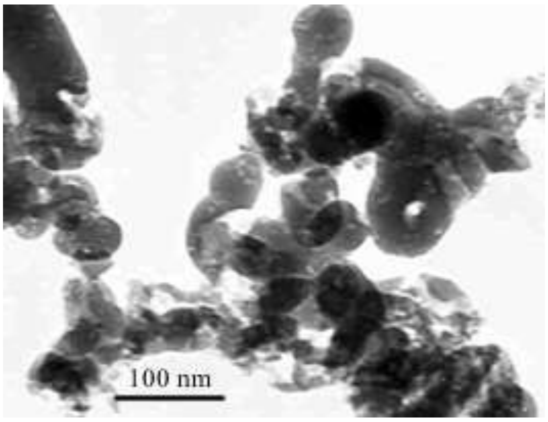

Fig. TEM microphotography of nanoparticles

Hysteresis loops recorded at the temperature of 300 K for the samples sintered at three different temperatures. The crystal structure, surface morphology, and magnetic characteristics of nanoparticles were studied by X-ray diffraction analysis, transmission electron microscopy, and vibrational magnetometry.

Scattering of conduction electrons on the W(001) surface covered with deuterium monolayer: the role of surface electronic states

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Substantial increasing of specularity of surface scattering of conduction electrons was found after covering the atomic clean W(001)-$(\sqrt{2}\times\sqrt{2})R45^{\circ}$ surface with ordered deuterium monolayer. UHV experiments were performed using the technique based on measurements of adsorption-induced changes of transversal magnetoresistance (MR) of thin ($\approx$100 μm) single crystal W(001) plates being under classical galvanomagnetic size effect [1] conditions (Fig. 1). To analyze experimental findings Fermi contours of surface electronic states at the atomic clean W(001)-$(\sqrt{2}\times\sqrt{2})R45^{\circ}$ and the monolayer covered W(001)-2D surfaces were calculated by the DFT method (Fig. 2).

Transformation of the W(001)-$(\sqrt{2}\times\sqrt{2})R45^{\circ}$ Fermi-contours caused by formation of deuterium monolayer W(001)-2D was shown to result in breaking conservation laws of energy and tangential component of crystal momentum for part of conduction electrons transition between surface and bulk electronic states. It leads to double reduction of probability of the transitions and increase the total specularity of conduction electrons surface scattering.

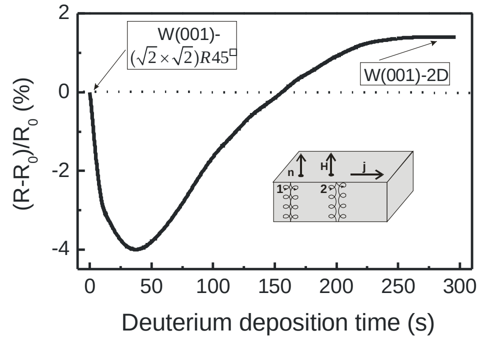

Fig. 1. MR changes of the W(001) plate induced by deuterium adsorption at $T \approx 5$ K (R_0 – MR of the plate with atomically clean surfaces). Insert depicts schematic of the experiment and trajectories of conduction electrons: *1* – specular surface scattering, *2* – diffuse surface scattering

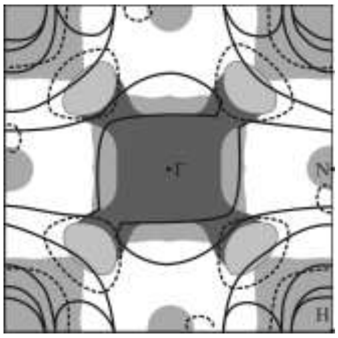

Fig. 2. Shadow projection of the W Fermi-surface onto (001) plane (gray regions) and calculated Fermi-contours of surface electronic states for the W(100)-$(\sqrt{2}\times\sqrt{2})R45^{\circ}$ surface (solid lines) and the W(001)-2D surface (dashed lines)

1. O.A. Panchenko, P.P. Lutsishin, S.V. Sologub, Prog. Surf. Sci. **96** (2002) 193.

Effects of ions on the properties of aqueous suspensions of nanosilica

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Addition of electrolytes to aqueous suspension of nanosilica leads to reorganization of both solvent (dispersion medium) and dispersion phase. Ions of a small size but great charge such as Li^+, Na^+, Be^{2+}, Mg^{2+} have stronger structurization effects on water than larger ions with smaller charges such as NH_4^+, Cl^-, Br^-, I^-, NO_3^-, ClO_4^-. In the aqueous dispersion medium, the rearrangement of the solvate shells of the ions could occur due to their interaction with nanoparticles and these effects depend strongly on the morphology and surface structure of nanoparticles. The aim of this study was to determine the ions influence on the formation of coagulation contacts between silica nanoparticles and the rheological properties of the suspensions with the presence of various electrolytes.

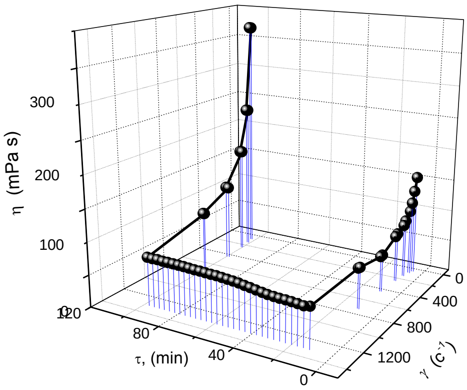

Fig. The dependence of viscosity on shear rate vs. time for 10 wt.% silica suspension with 0.1 M NaI in 10 days

The rheological properties of the dispersions were studied using a rotational viscometer Rheotest 2.1 (cylinder system S/N) at a shear rate of 9-1312.2 s^{-1}. The effect of electrolytes on the viscosity of the dispersion significantly varies. $NaNO_3$ and NaCl increase the solution viscosity, but NaI decreases the viscosity in comparison to the distilled water. The viscosity of the nanosilica suspensions with the presence of electrolytes is higher than that without addition of any salt. With the presence of sodium salts with different anions, the effective viscosity of nanosilica suspensions increases in the series $I^- < NO_3^- < Cl^-$ due to the formation of a larger number of coagulation contacts between the particles. All the studied suspensions demonstrate typical thixotropic behaviour in the range of 2.5-10 wt.% (Fig.). This is manifested in destruction of dispersion structure during rheological studies with increasing shear rate (γ) and restoring it with reducing shear rate. At nanosilica concentrations > 7.5 wt.% with the presence of electrolytes, the rheopexy is observed in 3 days of aging. For nanosilica suspension prepared in distilled water without electrolytes, the gel was not formed and the system remains free-dispersed during, at least, 14 days.

The method of applying a protective hydrophobic coating on the surface of CsI scintillator

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CsI:Tl crystals are widely used in science and technology as efficient scintillators for the registration and identification of charged particles by atomic number and mass. Due to the significant difference in the signal decay time from gamma quanta, alpha particles, light and heavy ions, the scintillation material CsI:Tl makes it possible to confidently distinguish between particles in the shape of an impulse. The problem of using these crystals is the state of the surface and the appearance of a dead layer near the surface. To ensure the stability of the characteristics, the working surface of the detector is protected by the film, despite the partial absorption of particle energy in the coating. The standard alpha detector consists of a 0.35 mm CsI:Tl crystal that is glued to a glass window. At the entrance window for radiation, a varnish (transparent solution of nitrocellulose in acetone) is deposited in a thickness of 5 microns.

The purpose of our work was to develop a method of applying a protective coating to the entrance surface of scintillator to reduce the thickness of the hydrophobic film and to improve the spectrometric characteristics of the detector in the registration of α-radiation. Fluoroplastic varnish is used as a protective coating, which allows improving the hydrophobic properties of the protective film, due to the low water absorption of lacquer. The high transparency of the varnish provides good optical characteristics and photo stability protective coating. The thickness of the coating from fluoroplastic varnish can be significantly reduced due to the addition of ethyl acetate to its composition. When the solvent is added to the composition of the fluoroplastic varnish, the viscosity of the composition changes, so that the coating is evenly applied to the surface of the crystal. However, high chemical inertness and low surface fluoroplastic energy are responsible for the low adhesion of the coating to the surface of the crystal. It has been shown that treatment of polished surface of the CsI:Tl crystal in hexamethyldisilazane vapors can increase the adhesion of the fluoroplastic coating to the surface of the crystal due to chemical reactions forming a thin layer of hexamethyldiisiloxane on the surface, which is a promoter of adhesion for hydrophobic film of 2 μm in thickness. It has been shown that the light output of a detector is increased by 400 channels compared to prototype, and the energy resolution is improved from 6.27 to 5.03 %.

Transformation of the magnetic properties of synthetic goethite and hematite in an aqueous medium

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The aim of this study is to investigate the phase transformations of synthetic hematite and goethite nanoparticles in aqueous medium under the influence of thermal and microwave heating. Sample of synthetic goethite was obtained by mixing iron(III) nitrate and potassium hydroxide solutions in water. The suspension was heated in a thermostat, in a closed flask, for 60 hours at 70°C. Sample of synthetic hematite was obtained by heating of synthetic lepidocrocyte at 650° C for 20 minutes. Transformation of samples took place under the influence of two heat sources: thermal and microwave. A solution of iron(II) sulfate was added to initial sample of synthetic goethite or hematite, during the process. After that, the reaction was started by adding ammonium hydroxide. Then the solution was incubated in a reactor at T = 98°C for 30 min. The same reagents were used for the the process with the use of microwave heating, but the incubation of the mixture occurred within 15 minutes (using a microwave frequency of 2450 MHz).

Phase composition of initial samples was determined by X-ray diffraction (X-ray diffractometer DRON-UM1). Measurement of the saturation magnetization during the transformation process occurred on an expressive measurement device for the magnetization of ores and magnetic materials. The X-ray diffraction analysis showed that the initial samples were presented as pure goethite (*d*-spacing (Å) 4.16, 3.37, 2.67, 2.57, 2.43, 2.25, 2.19, 2.04, 1.91, 1.79, 1.71, 1.56, 1.45 and 1.41) and hematite (*d*-spacing (Å) 3.67, 2.69, 2.51, 2.20, 1.83, 1.69, 1.59, 1.48 and 1.45). Saturation magnetization for initial samples was < 1 A·m^2/кg.

After transformation under the influence of thermal heating, the value of the saturation magnetization for a sample obtained from synthetic goethite was 16 A·m^2/kg, and for synthetic hematite, 18 A·m^2/kg. After transformation under the influence of microwave heating slightly higher values of saturation magnetization were obtained: for a sample from synthetic goethite – 18 A·m^2/kg, and for a sample from synthetic hematite - 19 A·m^2/kg. Consequently, the saturation magnetization of samples increased as magnetic minerals (magnetite) formed in the transformation.

Size-controlled synthesis of nanocrystalline silicon dioxide by Stöber process

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In recent years, silica nanoparticles become one of the most important material for hydrophobic coatings, catalysis, pigments, stabilizers, drug delivery and other medical and industry applications [1]. The size of the silica particles and average monodispersity have great influence on the property of these products. Therefore, the aim of this study was to compile an algorithm for obtaining a high degree of monodispersity of Stöber particles.

Stöber process is the simplest and most effective method to prepare monodisperse silica spheres with a size of 30–60 nm. During the hydrolysis reaction, the ethoxy groups of TEOS react with the water molecules that results in formation of the intermediate $Si(OC_2H_5)_{4-X}(OH)_X$ with hydroxyl group substituting ethoxy groups [2]. Ammonia works as a basic catalyst to this reaction.

Ammonium hydroxide (NH_3, 25%, A.R.), purchased from Sigma Aldrich, ethanol (99.9%, MOS) and TEOS (98%, A.R.) are obtained via direct reaction of MgSi and dry ethanol [3]. The purity control was carried out using GCMS (Agilent 7890A). The monodispersity of the particle size was maintained over a wide range of TEOS, H_2O, and NH_3 concentrations. All reagents are mixed by magnetic stirrer and left 24 hours at room temperature. The solution was then centrifuged to obtain a solid pellet of particles, which was dried at 50^{o}C. Systematic variation of reaction parameters allows to control formation of silica nanoparticles. Obtained samples at different conditions were investigated by TEM. According to TEM images the particle size increases with TEOS concentration. Hydrolysis and condensation become faster when NH_3 concentration is increased. Further investigation for the size distribution was carried out using AFM. AFM images show the spherical shape of the nanoparticles with a diameter in rage of 30-40 nm according to the variation. Comparison both of AFM and TEM images gives more accurate information about size distribution.

Systematic variation of reagents concentrations and grain size control allows to obtain a silica nanoparticles with given size and dispersity.

1. S.K. Park, K.D. Kim, H.T. Kim, Colloids Surf. A. **197** (2002) 7.
2. Ismail A.M. Ibrahim, A.A.F. Zikry. J. Am. Sci. **6**(11) (2010).
3. Ashurov *et al*. US9156861B2, Method for preparing trialkoxysilane, 2015.

Influence of nitrogen implanted in titania-stainless steel on photocatalytic activity

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Aromatic compounds are widely used in many industries and they have been considered common pollutants in industrial or agricultural wastewater, gaseous emissions [1].

These substracts contaminated by benzene compounds threatens the public health and has negative impacts on the ecosystems. New alternative treatment way of contamined wastewater instead of chemical oxidation and activated carbon adsorption is photocatalysis. Using of powder catalysts has some difficulties such as its removing after process, especially in aqueous solutions. On this basis, supported catalysts devoid of this disadvantage.

Previous part of work concerned on N-doped TiO_2 supported on silica. Actual study was focused on metal foil and ceramic composites, which completely eliminate the stage of catalyst filtering and separation.

The low temperature ion implantation is one of the useful methods for obtaining thin films of Ti, Sn, Zn and as well as their oxides on metal foil and Al-Si-O ceramic. In this study, the implantation dose was 10^{18} ions/cm^2 in nitrogen atmosphere.

The formation of Me-O_x-N_y nanolayers (100-200 nm) in dependence on post-treatment temperature was observed by SEM.

The UV-Vis spectroscopy shown shifts to the visible range for all of the samples calcined at 300-350 °C on air.

The photocatalytic activity of the samples was studied in gaseous and water solutions using UV or Vis irradiations in closed circulating system. It was shown that the post-treatment temperature strongly influences on benzene degradation rate.

Acknowledgements
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1. H. Dewidar *et al*., Uv. J. Chem. Health Safety. (2017) in press.

The effect of carbon nanotubes on the enzymatic activity of the yeast cells *Saccharomyces cerevisiae*

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The effect of the presence of carbon nanotubes (CNTs) in the aqueous suspension of *Saccharomyces cerevisiae* yeast cells (Saf Levier) in the concentration region (0-1%) on the kinetics of the heat release by cellular organisms during the fermentation process under the anaerobic conditions of endogenous metabolism was studied. A differential microcalorimeter (DMC) was used in the isothermal regime (295 ± 0.5 K). The sensitivity of the DMC on the heat flux was 10^{-6} W.

In contrast to earlier studies of the vital activity of yeast cells in an aqueous medium in the presence of nanoparticles of granular materials, there is a marked increase in the rate of cell hydration (its release accelerates from the anabiotic state), and the rate of quasi-chemical reaction of the enzymatic process decreases.

First of all, this is due to the high degree of anisodiametry and the anisotropy of CNTs in terms of heat and thermal diffusivity, as well as their significantly higher values in comparison with those for water.

An analysis of the effective thermal conductivity of a colloidal aqueous solution of CNTs was carried out on the basis of calculations based on the relations of the theory of generalized conductivity using a model with closed elongated inclusions of an anisotropic structure under conditions of both their orientation and an arbitrary undirected state.

The calculation shows that with the orientation of the nanotubes, the thermal conductivity can increase substantially in comparison with their undirected state. In this connection, at the cell-solution interface, the transfer of the energy released by the cell increases substantially due to a corresponding increase in the thermal conductivity of the habitat.

These changes in the environment, in accordance with the general principle of Le Chatelier-Brown's nature, force the cellular organism to lower the activity, which is manifested in the concentration dependence of the intensity of heat release and, consequently, enzymatic activity.

Formation of BeO on molybdenum (110) surface

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The interaction of oxygen with beryllium surfaces is of much interest due to the role of beryllium as a plasma facing material in experimental fusion reactors. Beryllium has advantages, including a low Z number and affinity towards oxygen and water vapor, allowing it to act as a getter for residual gases in the plasma vessel. Detailed understanding of the interaction of oxygen with transition metal surfaces is therefore essential for further progress in the development of layered and nanostructure materials with desirable properties.

The experiment was conducted in an ultra-high vacuum system (10^{-11} Torr) using the following methods: temperature-programmed desorption (TPD) with mass spectrometric detection (QMS), isothermal-desorption (ID), Auger electron spectroscopy (AES) and by the molecular beam (MB) method. It allowed us to comprehensively investigate the adsorption-desorption processes on the surface, *in situ*.

During the experimental study of the adsorption interaction of oxygen molecules with the nanolayer berilium on the surface of Mo(110) the mechanism of adsorption and the chemical state of the adsorbate on the surface was established. In the interaction of molecular oxygen from Be/Mo(110), beryllium is oxidized and formed BeO even at $T_s = 80$ K. At the Auger spectrum, peak satellites (96, 92 eV) of main peak Be (104 eV), indicating the surface oxidation. The increase in the exposure of O_2 to the Be/Mo(110) is accompanied by the development and chemical shift of the Auger peak oxygen ($512 \rightarrow 509$ eV), and the peak of metallic beryllium (104 eV) gradually disappears with the growth of the oxide layer of beryllium (96 eV). Complex results from MB, AES and TPD showed that the layer of oxide beryllium is formed already at an exposure in the atmosphere of oxygen ~ 10 Langmuir.

The results obtained by TPD and ID methods with mass spectrometric detection of desorption products on two quadrupole mass spectrometers (QMS) showed that the main desorption products from BeO/Mo (110) are atoms of beryllium and oxygen (BeO - not detected). In the TPD spectra, three peaks of the desorption of Be atoms are observed at various temperatures of 1250, 1570, and 1780 K. Moreover, the desorption peak at 1250 K corresponds to the non-oxidized metallic Be, and at 1780 K, simultaneous desorption of atomic oxygen and beryllium atoms is observed. This indicates that the BeO oxide layer dissociates on the surface at $T_s > 1550$ K, and has a higher binding energy with the surface Mo(110) than the metallic film of beryllium.

The formation of polysilsesquioxane-based materials with bifunctional surface layer

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The formation of bifunctional surface layer is an efficient instrument of tuning the properties of composite materials used as adsorbents for the removal of heavy and precious metal ions from water solutions [1]. Therefore, our research aimed to combine amino and mercapto groups in the surface layer of porous nanoparticles. We used modified Stöber technique [2, 3] to synthesize polysilsesquioxane particles using 1,2-*bis*(triethoxysilyl)ethane as a structuring agent. Due to the organic bridge, this bissilane promotes the formation of porous particles and improves access of target ions to the functional groups by increasing the distance between them. Meanwhile, the presence of two types of groups would provide different reaction sites on the surface.

As long as such materials are planned to be used as adsorbents we decided to introduce a magneto-sensitive component. The presence of magnetic core makes it possible to remove the sorbent from working solutions after sorption quickly and effectively, compared with conventional silica gel sorbents.

The materials properties were analyzed by a range of physical and chemical methods showing the formation of about 100 nm nanoparticles with well-developed porous structure, high surface area (350-600 m^2/g) and having the target amino- and mercaptopropyl groups on the surface. The study of the sorption properties shows the possibility of using such materials as sorbents of heavy metal ions.

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1. V.V. Tomina, I.V. Melnyk, Y.L. Zub *et al.*, Beilstein J. Nanotechnol. **8** (2017) 334.
2. N.V. Stolyarchuk, M. Barczak, I.V. Melnyk, Yu.L. Zub, Nanophysics, Nanophotonics, Surface Studies, and Applications. **183** (2015) 415.
3. N.V. Stolyarchuk, H. Kolev, M. Kanuchova, R. Kellerd, M. Vaclavikova, I.V. Melnyk, Colloids Surf. A. **538** (2018) 694.

Antibacterial silica fillers and polymer composites for medical applications

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For polymer materials of medical purpose, antibacterial properties are required in many cases. The improvement of the biocidal characteristics of polymer composites can be achieved by the addition of fillers with effective antibacterial properties. The results of the synthesis of polyurethane-urea (PUU), filled with Ag-containing nanosilica and the evaluation of the antibacterial effectiveness of the polymer composites are described. All the composites were studied using UV-Vis and FTIR spectroscopies and TEM methods.

Three samples of precipitated silica, modified by compounds of silver and copper, were used to fill the PUU polymer. Modified silica samples contained 2 wt.% Ag and 1 wt.% Cu (labeled as No.1), 1 wt.% Ag and 1 wt.% Cu (No.2), and 1 wt.% Ag (No.3). Hydrophilic polymeric composites based on polyurethane-urea with fragments of a copolymer of N-vinylpyrrolidone, vinyl acetate, vinyl alcohol and with a filler content of 1 wt.% were formed as films with a thickness of 0.2-0.3 mm. The antibacterial activity of the polymeric composites was determined by the Petri dish method using pharmacopeial strains of Gram-positive (*Bacillus subtilis* ATCC 6633 *Staphylococcus aureus* ATCC 6538, *S. epidermidis* ATCC 12228, *Micrococcus flavus* ATCC 10240), and Gram-negative bacteria (*Pseudomonas aeruginosa* ATCC 9027, *Escherichia coli* ATCC 25922, *Salmanella enterica* NCTC 6017, *Proteus vulgaris* ATCC 6896). It was found that a polymer film without a filler did not cause a delay in bacterial proliferation, whereas filled polymeric composites led to the formation of growth delay zones of bacteria of 13-31 mm in diameter. Thus, these polymeric composites based on polyurethane-urea and Ag-containing silica have effective antibactericidal properties.

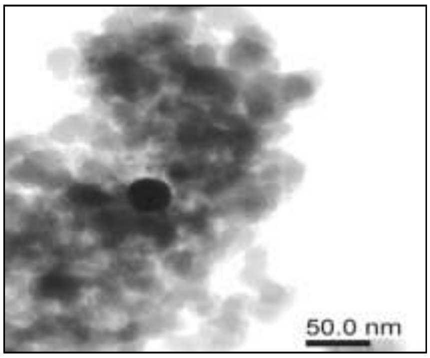

Fig. TEM image of sample No.3

Polymeric composites for biocompatible coatings

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The investigation goal was elaboration of effective carriers of biological active substrate and coatings for stents or scaffolds based on filled polymers or co-polymers. An ideal scaffold for biomedical applications as known should be a three-dimensional constitution that is highly porous to guarantee oxygen permeability, sufficient nutrient transport to the cells, and removal of waste products. Additionally, the scaffold should have mechanical properties suitable for the *in vivo* tissue at the site of implantation and should be easily connected to the vascular system of the host. Hydrogels are an important three-dimensional class of scaffolds used in tissue engineering, with their primary advantage being cell protection, which is possible because of their aqueous nature. As early as 1960, poly(2-hydroxyethylmethacrylate) (pHEMA) hydrogels had been successfully applied as biomedical materials in plastic surgery, ophthalmology, and drug delivery. pHEMA was the preferred choice of scaffold material, because its excellent mechanical properties and high hydrophilicity made it suitable for conversion into different architectures. Unfortunately, similar to other hydrogels, pHEMA hydrogels are not biodegradable and are typically inserted into the body by surgical means, limiting their widespread application. Chitosan, a biodegradable, naturally occurring polymer, has drawn considerable attention in recent years as scaffolding material in tissue engineering and regenerative medicine. Chitosan is especially attractive as a bone scaffold material because it supports the attachment and proliferation of osteoblast cells as well as formation of mineralized bone matrix.

In this review, we discuss the unique properties of chitosan and pHEMA films as a scaffolding material. We present the common methods for fabrication and characterization of scaffolds, and discuss the influence of material preparation on polymeric composite properties such as thermal degradation, mechanical strength, conductivity. Several types of polymeric materials based on chitosan or/and 2-hydroxyethylmethacrylate (HEMA) and carbon nanotubes (MWCNT) were synthesized and tested. Polymeric composites have been prepared by despergation of carbon nanotubes into the monomer HEMA or the chitosan solution. Obtained materials were characterized using FTIR, ATR, DSC and TMA analysis. Beside this all materials were tested on conductivity.

Synthesis of multilayer azagraphene and carbon nitride oxide

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As the promising photocatalyst for green energy, graphite-like carbon nitride and its nanostructured and doped derivatives attract special attention [1]. In our laboratory a new substance – carbon nitride oxide (g-C_3N_4)O was synthesized by gas phase method under the special reactionary conditions of the pyrolysis of melamine [2], urea [3] and cyanuric acid-urea mixture. For the first time at the reduction of (g-C_3N_4)O by hydroquinone, the reduced carbon nitride (or reduced multi-layer azagraphene) is obtained [4]. According to the results of chemical analysis and IR spectrometry (Fig. *b*) the chemical bonds between atoms in a heteroatomic plane of reduced carbon nitride (RCN) correspond to the bonds in a synthesized carbon nitride (SCN). Figure *c* shows schematic atomic model of one layer of SCN (the in-plane distance between the heptazine fragments (C_6N_7) d=0.714 nm). In connection with a break of some C–N bonds, in one layer of carbon nitride oxide (CNO) the in-plane distance increases to d=0.818 nm. After reduction (and consequently removing oxygen-containing groups) in-plane distance in a heptazine monolayer of the reduced carbon nitride (RCN) again decreases to d=0.714. However, RCN, which consists of poorly connected heteroatomic azagraphene layers, has a significantly larger (on 0.09 nm) interplanar distance between the adjacent nitrogen-carbon layers than interplanar distance between the layers of SCN (Fig. *a*).

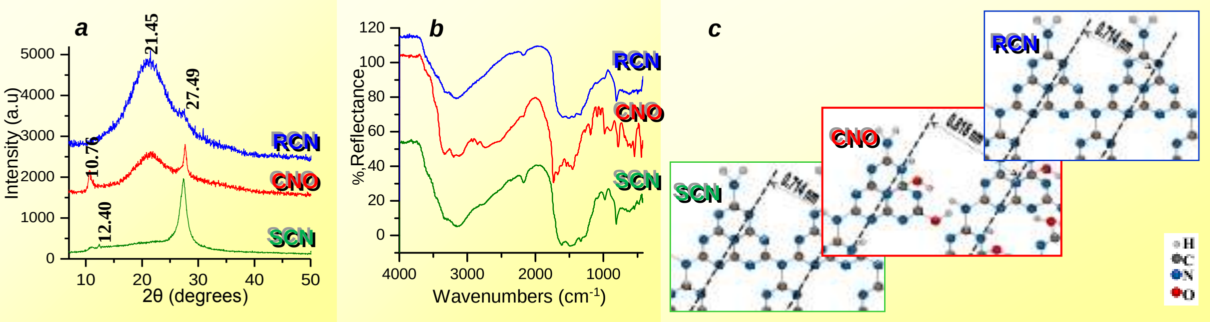

Fig. XRD patterns (*a*), IR spectra (*b*) and schematic atomic models of one layer (*c*) of reduced carbon nitride (RCN), carbon nitride oxide (CNO) and synthesized carbon nitride (SCN)

1. W.J. Ong, Front. Mater. **4** (2017) 10.
2. A. Kharlamov, M. Bondarenko, G. Kharlamova, Diamond Relat. Mater. **61** (2016) 46.
3. A. Kharlamov, M. Bondarenko, G. Kharlamova *et al*, Diamond Relat. Mater. **66** (2016) 16.
4. A. Kharlamov, M. Bondarenko, G. Kharlamova, J. Solid State Chem. **241** (2016) 115.

Synthesis carbon nitride films onto Ti substrate by thermal CVD melamine

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The problem of efficiently obtaining of hydrogen through photoelectrochemical water splitting is one of the most promising areas of renewable energy. Titanium dioxide is one of the most common photoanode materials for this process, its only drawback is the lack of activity in the visible range of solar radiation [1]. A polymer-like semiconductor, carbon nitride, can act as photoelectrode material for the evolution of hydrogen from water in visible light. In the present experiment thin films of C_3N_4 were deposited on the surface of Ti substrates in two ways: by CVD method and by deposition from an aqueous suspension of pre-synthesized (from melamine according to the method developed by us earlier [2]) graphitic carbon nitride. Titanium foil 0.5 mm thick and about 0.5 cm^2 was used as the substrate. The synthesis of films by the CVD method was carried out in the temperature range 500-550°C, melamine was used as a precursor. In the diffractograms of all the samples (Fig. *a*), only two reflexes are present at 2θ = 12.46 and 27.49°, which are characteristic for graphitic carbon nitride. Due to the low thickness of the g-C_3N_4 coating (submicron according to the scanning electron microscopy (SEM) data (Fig. *c*, d), the diffraction line at 2θ=27.49°, which characterizes the interplanar distance (0.324 nm) between adjacent nitrogen-carbon planes, is much less intense, than a line of powdered carbon nitride. In the IR spectra of all three samples (Fig. *b*) there are both an absorption band at 810 cm^{-1} and a series of distinct intense bands in the 1200-1650 cm^{-1} region, which are characteristic for the IR spectrum of graphitic carbon nitride g-C_3N_4.

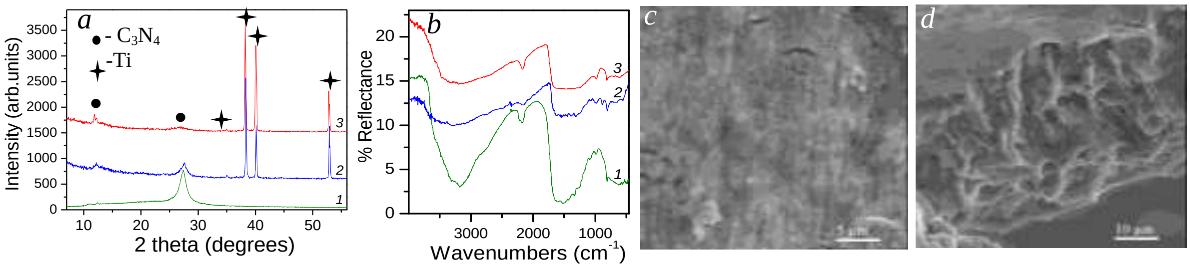

Fig. XRD patterns (*a*) and IR spectra (*b*) of: *1* – g-C_3N_4 powder, g-C_3N_4 films obtained: *2* – by CVD method, *3* – by method of deposition from aqueous suspension; SEM images of g-C_3N_4 film obtained by CVD method (*c*) and the edge of g-C_3N_4 film-coated Ti substrate (*d*)

1. D. Danko, P. Silenko, A. Shlapak *et al.*, Sol. Energy Mater. Sol. Cells 114 (2013) 172.
2. A. Kharlamov, M. Bondarenko, G. Kharlamova, Diamond Relat. Mater. **61** (2016) 46.

Photocatalytic properties of S/TiO_2 nanocomposites

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Titanium dioxide is known to be used widely as a photocatalyst. Nowadays researchers paid attention to employing techniques of TiO_2 doping with different elements, such as N, S, C, F *etc*. This expedient leads to arriving of light absorption in the visible domain of spectra, the phenomenon being connected with the emergence of new electronic levels above the valence band of TiO_2. Thus, the aim of our work was to obtain and characterize composite materials based on titanium dioxide and sulfur with enhanced photocatalytic activity under UV and visible irradiation.

Nanocomposite materials were obtained by thermal hydrolysis using titanium ethylate with addition of thiourea. Samples were designated as S/TiO_2 (sulfur content being varied). Powders were studied by X-ray diffraction, scanning electron microscopy, transmission electron microscopy, sorption studies using BET interpretation and IR spectroscopy. Photocatalytic activity was studied using model reaction of safranin T cationic dye destruction in water solutions under ultraviolet and visible irradiation.

X-ray analysis revealed the phase of anatase and rutile in all the composites. It was established that composites consist of crystallites with size varying from 9 to 11 nm. Analysis of nitrogen sorption–desorption isotherms for the synthesized samples showed the presence of a hysteresis loop which is the evidence for mesoporous structure of the powders. The isotherms correspond to type IV of IUPAC classification for mesoporous materials. Increasing of sulfur content in the samples leads to increasing of their specific surface and mean pore volume.

Nanocomposite samples showed higher photocatalytic activity in the destruction of safranine T organic dye under UV and visible irradiation compared to pure titanium dioxide. Increase of photocatalytic activity of modified samples may be connected with the inhibition of the recombination of photogenerated electrons and holes due to efficient phase separation of charge.

Analysis for thermal decomposition of calcite biocrystalline structures from bird's hatching and food eggs

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One of the important problems in poultry is the problem of the strength of biocrystalline eggshell structures of the chicken eggs both food and hatching. Until now, there is no nondestructive method of analysis, which makes it possible to unambiguously predict the strength parameters of the eggs. The aim of our work is to study the relationship between the macrostructure of food and hutching chicken eggs and the dynamics of CO_2 release during the thermal destruction of shell samples by the TPD-MS.

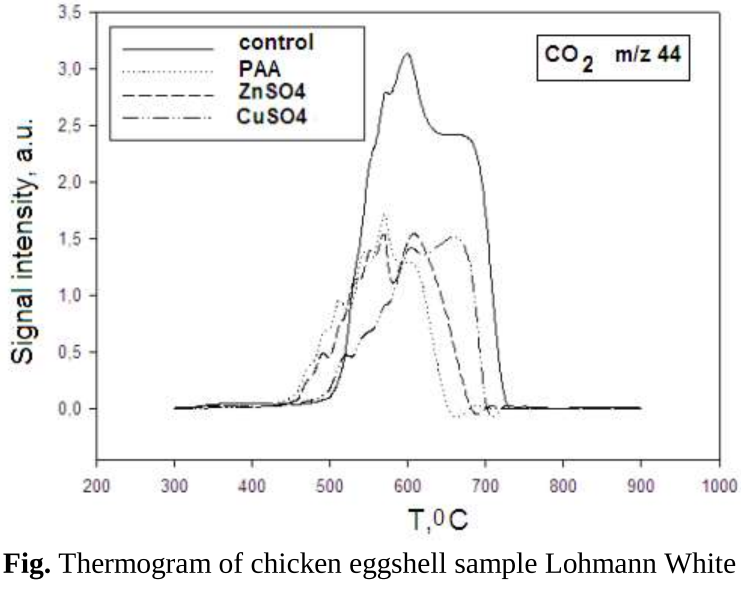

Fig. Thermogram of chicken eggshell sample Lohmann White

It is shown (Fig.) that there is a significant effect on the characteristics of thermograms of eggshell chicken eggs samples of both native and exposed biocidal chemical agents (peroxide compounds (PAA), heavy metal salts (Zn, Cu).

Structure and properties of nanofilled microfibrillary threads

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One of the effective methods for modifying polymer materials is the development of composites in which the disperse phase forms micro- or nanofibrils in a dispersion medium - microfibrillary (MFC) and nanofibrillary (NFC) composites respectively. Formation of *in situ* fibrils in a mixture of polymers allows the production of ultra thin fibers by extraction of a matrix polymer with MFC or NFC.

The purpose of the work is to study the properties of monofilament and complex threads based on PP microfibers, formed from mixtures of polypropylene/copolyamide (PP/CPA), filled with nano-additive Al_2O_3.

For research, mixtures were used PP/CPA composition 30/70 wt.% and nano-filled with aluminum oxide with a specific surface of 109 m^2/g. The content of Al_2O_3 was (0.1÷3.0) wt.%. The morphology of extrudates of mixtures was evaluated by the method of images analysis. The equivalent diameter (D_e) and shape factor (SF) of the particle disperse phase were determined. Monofilaments were formed on a laboratory bench. Complex threads were obtained by removing CPA with an aqueous solution of ethyl alcohol.

Microscopic studies have shown that matrix-fibrillar morphology is formed in all studied mixtures. Addition (0.1÷3.0) wt.% Al_2O_3 in the melt contributes to the improvement of the microstructure of extrudates. In comparison with the initial mixture, the proportion of particles with D_e (1÷2) μm increases ~ 3 times, increases the uniformity of their distribution and decreases the number of large agglomerates. The maximum effect is achieved with the content of Al_2O_3 in a mixture of 1.0 wt.%. For most particles, the SF is within the range of 0.8÷0.9. The mechanical properties of threads formed from mixtures of polymers are determined by the type of disperse phase structure in a dispersion medium. The formation of PP fibrils *in situ* in the CPA matrix provides for increasing the mechanical characteristics of the monofilaments through the process of self-reinforcement. The presence of Al_2O_3 in the structure of mono- and complex filaments contributes to the further improvement of their properties, which is due to the formation of the more perfect matrix-fibrillar morphology. With an Al_2O_3 content of 1.0 wt.%, the number of nano-filled PP microfibrils with diameters of 1.0÷4.0 μm increases to 82%. It is almost 2 times higher than that of the original mixture. Complex threads formed from a mixture of $PP/CPA/Al_2O_3$ of 30/70/1 wt.%, have maximum strength and resistance to deformation, and can be used for special textile products.

New antifouling paint containing polymeric biocide polyhexamethylene guanidine molybdate

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New promising low-cost and low toxic polymeric biocide PHMG molybdate has been synthesized. The obtained cationic polymer is insoluble in paint solvents and has limited water solubility. Commercial ship paint XC-413 (Ukraine) designed for the protection of underwater metallic constructions against corrosion was used in this study. The paint was modified with polymeric biocide by its dispersion as solid pigment in a concentration of 5% (w/w).

The stainless steel bars were coated with XC-413/PHMG molybdate paint (total coating thickness 300 ± 10 μm) and tested for antifouling properties. The adhesion of both control and modified coatings onto the substrates determined in accordance with ASTM D 3359, method B was found to have similar values of 1 point (5 B). The results of corrosion testing in salt spray chamber for 260 hours (ASTM B 117-03 Standart Practice for Operating Solt Spray (Fog) Apparatus) demonstrated good resistance of control panels (painted with neat XC-413), as well as XC-413/PHMG molybdate coated samples.

Preliminary studying have shown the antibiofilm activity of XC-413/PHMG molybdate coating against *Pseudomonas pseudoalcaligenes*, *Bacillus subtilis*, *Rhodococcus erytropolis* and *Stenotrophomonas maltophilia* bacterial test cultures. For the evaluation of antifouling properties, the painted steel substrates were immersed into Dnipro River for 228 days. It has been found that polymeric biocide impart the coating high resistance to bryozoan and zebra mussels which are the most aggressive macrofoulers in fresh water. Thus, PHMH molybdate modified coatings showed 40-fold reduction of total biomass formed by Bryozoa and 90-fold reduction of Dreissenidae fouling biomass, comparatively to control substrates surface.

The leaching rate of PHMG molybdate from the coating was found to be similar to those for conventional booster biocides ranging from 5.7 $\mu g \cdot cm^{-2} \cdot d^{-1}$ at the initial stage to 2.2 $\mu g \cdot cm^{-2} \cdot d^{-1}$ at the steady state.

The pyrogenic synthesis of a complex metal-oxide catalyst for the growth of carbon nanotubes

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The functional scheme of obtaining a complex metal oxide catalyst for the production of carbon nanotubes by the method of high-temperature hydrolysis (pyrogenic synthesis) based on the use of hydrocarbon liquid or gaseous fuels for obtaining a high-temperature coolant, which causes thermal shock to the aqueous solution of metal salts, is developed. The nature of combustion of hydrocarbon fuels allows to control the temperature of combustion products in wide limits and provides the opportunity to organize the process of thermal cleavage and evaporation in an optimal way.

In Table shows the values of the surface area of catalysts obtained by aerosol and pyrene methods and the nanotubes obtained on them.

Table. Specific surface, determined by the method of heat loss desorption of argon

Sample	Catalyst AlFeMo	CNT nonpurified	CNT purified
Specific surface area, m^2/g	**42** (aerosol)	320	295
	67 (pyrogenic)	360	358

The specific surface area of the catalyst obtained by the pyrogenic method is greater than the surface of the catalyst obtained by the aerosol process by about 50%, which allows for obtaining carbon nanotubes with a larger yield.

The study of carbon nanotubes obtained by the pyrogenic method using electron microscopy (Fig.) and thermogravimetric analysis showed that they have a high quality and almost do not contain amorphous carbon.

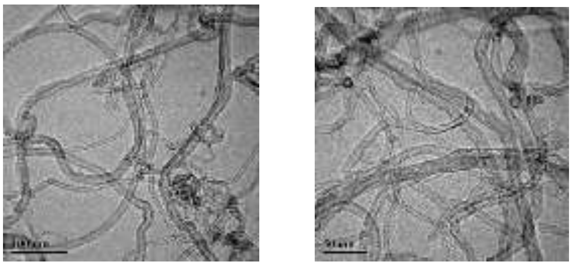

Fig. Electronic micrographs of multilayer nanotubes produced on a pyrogenic catalyst

Thus, it can be argued that the developed method of pyrogenic synthesis of the growth catalyst for carbon nanotubes allows the production of a highly dispersed catalyst to produce high-quality nanotubes with high yields.

Correlating structural changes and gas evolution during the thermal decomposition of mollusc shell

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Mollusc shells are very interesting objects for materials experts because the composite materials from which the shells consist are characterized by extraordinary strength. It has been showed by the X-ray diffraction method that calcite ($CaCO_3$) predominates in their composition. Surprisingly, calcite which is the main component of shells, is rather fragile. The perspective method that makes it possible to investigate the differences between biocomposites is temperature programmed desorption mass spectrometry (TPD-MS). The purpose of the study was to study some molluscs differing in strength of its shells (Fig.): *Mya arenaria* (*1*), *Mytilus galloprovincialis* (*2*) *Cypraea pantherina* (*3*).

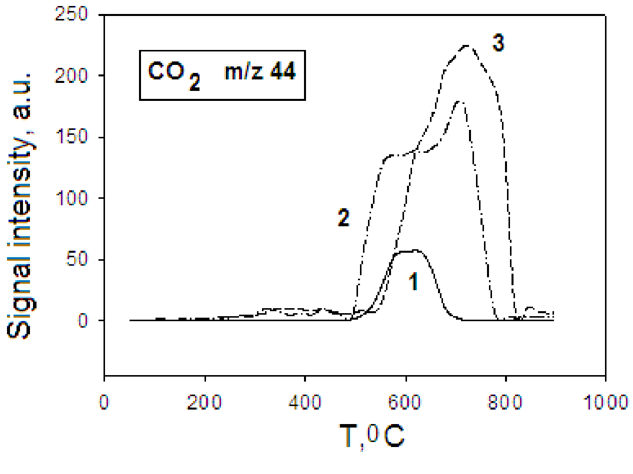

Fig. Thermograms of CO_2 ions obtained from the shells of *Mya arenaria* (*1*), *Mytilus galloprovincialis* (*2*), *Cypraea pantherina* (*3*)

The authors suggest the use of TPD-MS in a complex of analytical methods for determining the macrostructure peculiarities and shell strength of biocomposites.

Effect of electron transition kinetics on the photomotor velocity

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An expression for the average velocity of a semiconductor photomotor [1,2] has been obtained. A three-level model of the electron system of a photomotor with arbitrary transition rate constants has been considered (see Fig.), and the time dependences of its electronic level occupations have been calculated.

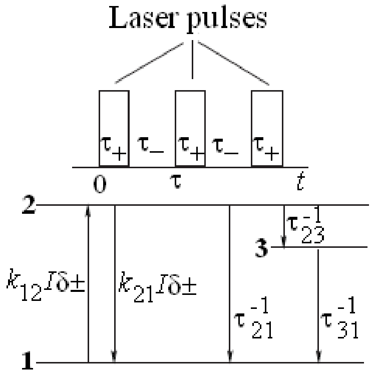

Fig. The effect of the cyclic sequence of laser pulses (at the top) on the three-level electron system of the semiconductor nanocluster photomotor (at the bottom). Level 1 corresponds to the ground electronic state of the system, level 2 to the state photoexcited by the laser tuned to resonance with the transition 1→2, and impurity level 3 describes the electronic state localized on the nanocluster surface. The possible electron transitions are marked with arrows, with the corresponding rate constants indicated

Level occupations changing with time determine the time dependence of the potential energy and the average velocity of the photomotor motion along the polar substrate. The optimum conditions of laser photoexcitation and the kinetic characteristics of electron transitions in the photomotor have been found which provide the maximum velocity of its directional motion.

1. M.L. Dekhtyar, V.M. Rozenbaum, L.I. Trakhtenberg, Russ. J. Phys. Chem. A **90** (2016) 1484.
2. V.M. Rozenbaum, M.L. Dekhtyar, S.H. Lin, L.I. Trakhtenberg, J. Chem. Phys. **145** (2016) 064110.

Analogues of Brooker's Merocyanine with varied donor-acceptor strength

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Derivatives of Brooker's Merocyanine have been investigated which possess different donors and acceptors and therefore vary their donor-acceptor-strength S_{DA} [1].

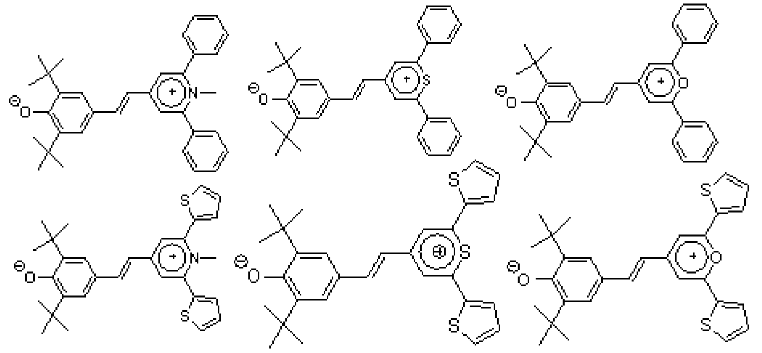

Fig. Structures of the investigated merocyanines (basic form)

The 00-energies of the merocyanines have been extracted from the spectra and compared. In basic conditions, where the neutral form is present, the absorption energies for all compounds are similar, whereas there is a large difference for acidic conditions. This behaviour could be explained by a model involving the S_{DA}-dependence of the excitation energy. This model can be generalized to describe two different classes of neutral chromophores with a certain degree of charge separation, namely merocyanine I (TICT) and merocyanine II (often betainic) compounds [1]. Merocyanines I are characterized by a medium polar aromatic ground state and a zwitterionic quinoid excited state and hence positive solvatochromism, whereas merocyanines II are formally characterized by a zwitterionic aromatic ground state and a less polar quinoid excited state and, accordingly, by negative solvatochromism. On increasing S_{DA} sufficiently, merocyanines II can, however, move to the so-called overcritical region with the excited state dominated by the zwitterionic valence bond structure. For many of the merocyanine II molecules investigated here, weakly positive solvatochromic behaviour is observed indicating that the ground state contains less of the zwitterionic valence bond wavefunction than the excited state and that these compounds belong to the overcritical region. The fluorescence spectra have been analyzed in terms of the Franck-Condon model and confirm these conclusions.

1. W. Rettig, M.L. Dekhtyar, A.I. Tolmachev, V.V. Kurdyukov, Chem. Het. Comp. **47** (2012) 1244.

Influence of nitrogen atoms introduced into the graphite-concrete carbon nanocluster on the H_2 adsorption

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Increasing requirements to the validity of modern storages of effective energy carriers cause an acute need in the materials capable to secure a wide range of operational conditions due to the specific chemical and physical properties of such systems. Because of the reserve depletion of energy sources, novadays dihydrogen is frequently thought to be an ideal altenative energy carrier. Nevertheless, a transition to prospective hydrogen energetics is impossible without developing valid methods of hydrogen producting, transpormation and storage in large quantities. One of the most prospective methods of hydrogen storage is its adsorption on carbonaceous materials [1]. In particular it can be recently obtained graphene with structural defects and doped heteroatoms (for instance, nitrogen atoms) as specific adsorption sites. The aim of this work is search for the natural lows of the interaction between hydrogen molecules and graphene-like planes bearing vacancies and nitrogen atoms formed due to elimination of substitution of one or some carbon atoms.

The calculations were carried out by density functional theory method with functional B3LYP, basis set 6-31G(d,p), and dispersion correction by Grimme [2] by means of USGAMESS program package [3].

An analysis of the results of quantum chemical studies has testified that the chemisorption energy for hydrogen on the graphene-like plane with mono- and diatomic vacancies and nitrogen atoms is for 50 to 120 kJ/mol greater than that for adsorption on an ideal (defect-free) graphene-like plane.

1. M. Pumera, Energy Environ. Sci. **4** (2011) 668.
2. S. Grimme, J. Antony, S. Ehrlich, H. Krieg, J. Chem. Phys. **132** (2010) 154104-1.
3. M.W. Schmidt, K.K. Baldridge, J.A. Boatz, *et al.*, J. Comput. Chem. **14** (1993) 1347.

Synthesis and properties of cryogels for medical applications

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Carriers based on cryogels can be used in medicine as biocontainers in the drug delivery systems for various purposes. Their use is particularly important for prolonged and controlled release of bioactive compounds. To achieve positive practical results in this direction, it is possible to develop the drug carriers with adjustable characteristics of the porosity, high biocompatibility, and appropriate degradation in the body. In this work, it is proposed to prepare the cryogels using solutions of polyvinyl alcohol (PVA) and chitosan as cryogel precursors using cryogelation processes under atmospheric and high pressure conditions. This choice was due to good biocompatibility and environmentality of the selected materials. Synthesized cryogels with a percentage ratio of PVA / chitosan as 3:1; 2:1; 1:1; 1:2; 1:3. In all cases, 25% glutaraldehyde was used as a crosslinking agent ranged in the molar ratio of 1 to 2 in relation to the amino groups of chitosan. The cryogel formation was carried out at -18 °C and atmospheric pressure or in cryobombs at *ca*. 1000 atm. The degree of swelling of high- and low-pressure cryogels in water and isotonic solution was determined. It has been established that the highest swelling is observed for samples 4 and 5 (Fig. 1, 2), in which the content of chitosan was predominated.

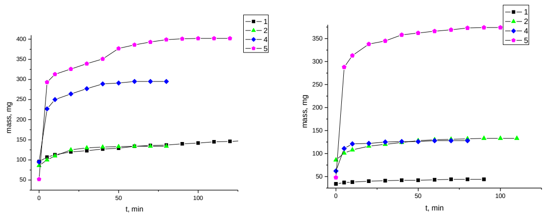

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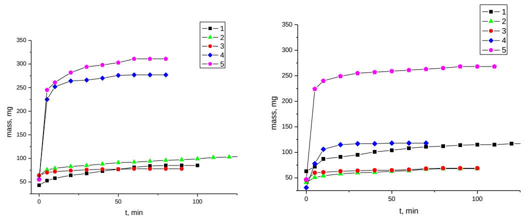
Fig. 1. Dependences of the degree of swelling of low-pressure cryogels in water (*1*) and isotonic solution (*2*) on time



1 2

Fig. 2. Dependences of the degree of swelling of high-pressure cryogels in water (*1*) and isotonic solution (*2*) on time

Infrared and thermogravimetric data of specimens characterized by the highest swelling rates were recorded and described.

As a result of the work, it was shown that the ratio of components and conditions of cryogelation (*e.g.*, at low and high pressure) allow us to prepare the cryogels with an appropriate degree of swelling and, consequently, to change the capacity of such "containers" and to study the kinetics of the process of release of medicinal preparations from their volume.

Influence of ultrasonic and mechanochemical treatment on reducing properties of CeO_2-MoO_3 systems

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Ce-Mo-O compositions are well known for ecological catalysis, and partial oxidation processes. The new methods for the preparation of oxide systems based on Ce and Mo may be ultrasonic (UST) and mechanochemical treatment (MChT), which allow to synthesize of composites with nano-sized particles.

The CeO_2-MoO_3-UST was synthesized in a dispersant UZDN-2T and CeO_2-MoO_3-MChT was synthesized in a ball planetary mill Pulverisette-6 (Fritsch). The obtained samples were characterized by XRD, ESR, adsorption of N_2, SEM, TEM, FTIR and catalytic tested in the reaction of bioethanol selective oxidation. The aim of this work was studies of UST and MChT impacts on reducing properties of Ce-Mo-O system. The reducing was carried out in a H_2-Ar mixture in the temperature range of 30-800°C at a heating rate of 10 °C/min.

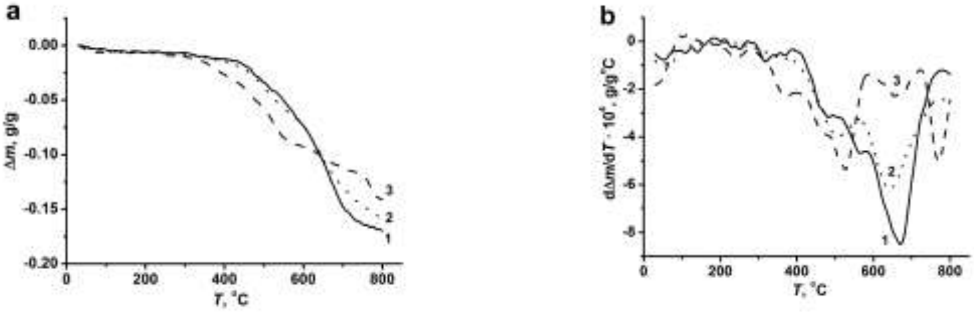

Fig. TG (*a*) and DTG (*b*) dependence of hydrogen reducing of samples: CeO_2–MoO_3 initial (*1*), CeO_2–MoO_3 UST (*2*) and CeO_2–MoO_3 MChT (*3*)

The TG/DTG dependences of the hydrogen reducing of the CeO_2-MoO_3 samples was shown in Fig. It was shown that the reducing of the initial sample CeO_2-MoO_3 begins at 400°C, that is 100°C less than the reducing of MoO_3. For the CeO_2-MoO_3-UST the reducing begins at 300 C with formation of MoO_2 (~550°C) and Mo (~750°C) that is clearly observed on the TG/DTG curves. It is found that the reducing of CeO_2-MoO_3-MChT begun at 250°C, and 65% of oxygen was removed from the sample up to 570°C. Thus, UST and MChT lead to the significant activation of the surface layer and the defects appearance in the samples structure, that accompanied by an increase of oxygen mobility and the ability to remove it already at 250-300°C as a result of controlled reducing.

The impact of reactive oxygen species on the surface structure of nanoceria

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Cerium oxide nanoparticles (CNPs) are of increasing interest for biomedical application because of their ability to quench reactive oxygen species similar to the antiradical activity of basic natural defense enzymes [1]. The latter believed to depend on Ce^{3+} / Ce^{4+} ratio at the particle surface, which could be used in electrochemical biosensing [2]. Recently developed optical sensor exploiting CNPs embedded in polyvinyl acetate, showed more stable and easy-to-use performance in peroxides detecting [3].

The objective of our work was to obtain CNPs capable of superoxide anion-radical quenching and to trace their optical characteristics as applied to potential free-radical sensing.

We prepared cerium dioxide nanoparticles via the simple chemical procedure of re-precipitation from cerium nitrate solution in alkaline medium and assessed the phase composition of the nanoceria by means of X-ray diffraction analysis.

Using xanthine oxidase / xanthine system as the source of superoxide anion radicals, we revealed superoxide mimetic activity of the CNPs accompanied by characteristic changes in their adsorption spectra. Under the superoxide anion radicals exposure the adsorption curve of the nanoceria had specific patterns comprised of smoothing the peak, which corresponds to Ce^{3+} (≈230 nm) and its replacement by the peak at ≈290 nm, which corresponds to Ce^{4+}.

Conclusion: the nanodispersed cerium dioxide acting as superoxide mimetic displays specific changes in Ce^{3+} / Ce^{4+} surface ratio under the impact of free radicals that results in characteristic shift of its absorption spectra.

1. G. Pulido-Reyes, I. Rodea-Palomares, S. Das *et al.*, Sci. Rep. **5** (2015)15613.
2. S. Sudipta, C. Hyoung, P. Swanand, M. Anjum, WIPO Patent Application WO/2006/130473.
3. N. Shehata, E. Samir, S. Gaballah, A. Hamed, A. Elrasheedy, Sensors. **16** (2016) 1371.

Semi-synthetic adsorbents based on montmorillonite and silica gel

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Over the past century there has been a dramatic increase in scientific reports due to the pollution problem of the water basin by organic and inorganic toxicants. In the new global economy, the development of modern cheap and effective sorption materials has become a central issue. We consider a semi-synthetic sorbent derived from a natural clay mineral, montmorillonite, and a sodium silicate solution as a perspective. The composites obtained by this method may have a solid microporous frame structure since the alumina-silicate montmorillonite particles are bound together by silica molecules formed as a result of the sodium silicate hydrolysis.

Samples of the triple system montmorillonite–sodium silicate–water were studied. All the samples are characterized by the 3% by weight content of montmorillonite. The content of sodium silicate in the system is in the 0.1 - 10% by weight range (in recalculation on SiO_2).

The processes of structure formation in the system were investigated in terms of rheological and X-ray diffraction analysis. Sorption properties of obtained samples were studied in static conditions using model solutions. Organic dye (methylene blue) and heavy metal ions (Co^{2+}) were used as pollutants.

An extremal character (an extremum at 0.1-1% SiO_2 content) in the limiting shear stress and plastic viscosity dependence of the montmorillonite–sodium silicate–water system was established. It can be explained with the formation of siloxane bonds. Only amorphous silica is fixed on the XRD patterns if the content of sodium silicate in triple system is more than 1%. The resulting semi-synthetic material retains its sorption properties in the removal of methylene blue (up to 450 μmol/g) and Co^{2+} (up to 350 μmol/g).

It is proved that the use of sodium silicate as a modifier allows to obtain sufficiently effective and cheap semi-synthetic sorption materials for the removal of organic dyes and heavy metals from contaminated water. This study shines a light on the further investigations (the efficiency of these sorbents for the radionuclides removal).

Nanocrystallite growth activation energies of the apatite under isochronal thermal treatment

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The present work represents the calculations of nanocrystallite (NC) growth activation energy (AE) values related to the biogenic (BHA) and stoichiometric, synthetic hydroxyapatites (SSHA) (NPP "KERGAP", Kiev, Ukraine). Activation energy calculations were based on the previously published data on X-ray diffractometry (XRD) [1]. BHA samples were prepared from the highly mineralized bovine bone. Bone samples were studied both as a powder and oriented plates. SSHA substrates were in a finely dispersed powder form. In the calculations, raw data values were equal to the crystallinity (1/FWHM), and it was postulated that NC growth is controlled by a diffusion of the ion complexes. In so doing, an average crystallite size in the square of $\langle d\rangle^2 \sim D$, where D is the effective diffusion coefficient (EDC). The samples were annealed at temperatures in the range of 600...1100°C with a step of 100°C exposing to each fixed temperature value during 1 h. Arrhenius plots of the EDC were obtained. Extracted from the Arrenius plots, AE of NC growth in BHA value was found to be 2.59 eV and is consistent with those from ref. [2] obtained using XRD (1.90 eV), and Differential Scanning Calorimetry - DSC (2.84 eV), Thermal Gravimetric Analysis - TGA (2.35 eV) techniques (see [2] and references therein). Moreover, EA of NC growth in BHA is in correlation with that obtained using Thermal Programmed Desorption Mass Spectrometry - TPD MS technique based on the release of CO_3^{2-} at 976 K [3]. Data of [2] have the lesser value which the authors relate to peculiarities of the initial mineral nanocrystalline state. Value of AE in SSHA samples was found to be unexpected lower (of about an order of magnitude) than that obtained in [2]. Thus, realistic values of NC growth AE were obtained in apatites under isochronal thermal annealing using quite simple approximation. Two different possible mechanisms of the NC grain growth will be discussed in the report.

1. S.N. Danilchenko, A.V. Koropov, I.Yu. Protsenko, B. Sulkio-Cleff, L.F. Sukhodub, Cryst. Res. Technol. **41** (2006) 268.
2. C. Greenwood, K. Rogers, S. Beckett, J. Clement, J. Mater.Sci.: Mater.Med. **23** (2012) 2055S.
3. S.N. Danilchenko, V.A. Pokrovskiy, V.M. Bogatyrov, L.F. Sukhodub, B. Sulkio-Cleff, Cryst. Res.Technol. **40** (2005) 692.

Nanocomposites based on inorganic ion exchangers and carbon materials

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Advanced carbon nanomaterials are known to improve functional properties of polymers [1], particularly biopolymers [2], ceramics [3] *etc*. Moreover, the carbon additives impart new properties to mentioned substrates, for instance, electrical conductivity, catalytic activity, adsorption ability towards organics.

The method, which allows us to create nanocomposites consisting of sorbents of different nature, has been developed. The constituents are hydrated oxides of multivalent metals and carbon materials, such as activated carbon, carbon nanotubes, reduced and oxidized graphenes. The crude for preparation of pristine carbon is the wastes of sugar industry. The advantages of the nanocomposites over inorganic sorbents, such as oxides, phosphates, heteropolyacids *etc*., are ability to adsorb not only inorganic ions, but also organic compounds. As opposed to carbon materials, mechanical durability is attributed to the nanocomposites. In contradiction to graphenes and nanotubes, two-component materials could be obtained in a form of large granules (up to 1 mm), this gives a possibility to apply them to adsorption columns. Unlike known two-component adsorbents, homogeneous distribution of the carbon constituent through the inorganic matrix is achieved. This provides reproducibility of functional properties of the adsorbents.

The nanocomposites were investigated with methods of X-ray diffraction, IR spectroscopy, scanning and transmission electron microscopy. Hydrophilic and hydrophobic porosity was estimated with standard contact porosimetry similarly to [2]. The materials were recommended for simultaneous removal of molecular organic compounds and inorganic ions from water, biological liquids and industrial wastes, they can be also applied to membrane modification.

1. B.M. Gorelov, A.M. Gorb, O.I. Polovina, A.B. Nadtochiy, D.L. Starokadomskiy, S.V. Shulga, V.M. Ogenko, Nanosystems, Nanomaterials, Nanotechnologies. **14** (2016) 527.
2. Y.M. Shulga, S.A. Baskakov, Y.V. Baskakova, A.S. Lobach, E.N. Kabachkov, Y.M. Volfkovich, V.E. Sosenkin, N.Y. Shulga, S.I. Nefedkin, Y. Kumar, A. Michtchenko, J. Alloys and Compounds. **730** (2018) 88.
3. V.V. Goncharuk, L.V. Dubrovina, D.D. Kucheruk, A.O. Samsoni-Todorov, V.M. Ogenko, I.V. Dubrovin, J. Water Chem. Technol. **38** (2016) 34.

Adsorption of physiologically active substances by medical carbon adsorbents with different bulk density

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The main requirements for carbon hemosorbents are durability and absence of dusting of carbon granules, hemocompatibility, high sorption properties relative to toxins of different chemical nature and molecular weight. Earlier, uncoated spherical granular synthetic carbons SKN and SKS, which met above requirements even at high degrees of burn-off (up to 80%), were used in the medical practice of the CIS countries. At present, in Ukraine production of these activated carbons and medical adsorbents on their basis is discontinued for various reasons.

Processing technology of granular carbon adsorbent "Carbon" was developed at ISPE, NAS of Ukraine. Commercial activated carbon AquaCarb 607 C ("Chemviron Carbon", Belgium) based on coconut shell was activated in addition by steam-air mixture. The task of the present work was to find out the influence of burn-off or bulk density on the porous structure of "Carbon" and its sorption capacity in relation to amino acids (tryptophan and arginine), their metabolites (indole) and uremic toxins (creatinine).

Investigation of the porous structure of the adsorbent "Carbon" (bulk density is from 0.22 to 0.43 g/cm^3) showed that these materials are micro-mesoporous. It has been found that specific surface area and pore volume associated with adsorbent weight increase with decrease of its bulk density, and values of these parameters related to the volume have a maximum at bulk density of 0.35 g/cm^3. Kinetic data and sorption capacity of the "Carbon-0.35" adsorbent in relation to tryptophan, arginine, indole and creatinine (2.6, 1.8, 4.1 and 2.55 mmol/g, respectively) were obtained. Values of sorption capacity depend on hydrophobic properties of these compounds.

Observation of sample morphology by means of SEM demonstrates that use of steam-air mixture leads to decrease of the bulk density of carbon adsorbent due to formation of mesopores in its structure, volume of which depends on degree of material burn-off.

Thus, method of steam-air activation make it possible to retain high mechanical strength and low dust formation of uncoated carbon adsorbents. "Carbon-0.35" adsorbent is made as filling material for high-performance hemosorption columns ("Farmavit", Belarus) and is promising for the treatment of patients with liver disease.

Copolymerization and study of physicochemical properties of the microspheres based on aromatic thiols and DVB

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The copolymerization of two aromatic methacrylic derivatives of thiols: phenylthiomethacrylate (PSM) and naphthalenethiomethacrylate (NAFSM) with divinylbenzene (DVB) was used for the synthesis of cross-linked mesoporous microspheres. The suspension-emulsion polymerization in the presence of the pore-forming diluents, decan-1-ol and toluene was performed [1-3]. The porous structures of the obtained microspheres in the dry state were investigated by low-temperature nitrogen adsorption data. Their chemical structure was confirmed by ATR/FT-IR spectroscopy. The swelling properties of the obtained copolymers as well as their thermal properties as studied by DSC analysis were discussed in detail. The morphology of the obtained microspheres was visualized by optical microscope MORPHOLOGI G3 Malvern.

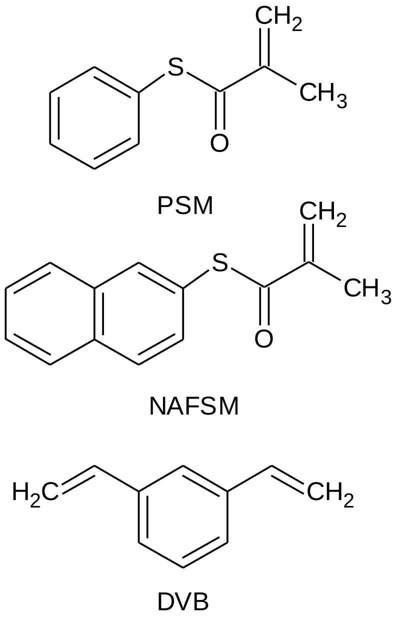
PSM
NAFSM
DVB

Fig. Chemical structure of the monomers used for copolymerization

1. B. Podkościelna, A. Bartnicki, B. Gawdzik B, J. Appl. Polym. Sci. **111** (2009) 1257.
2. B. Podkościelna, D. Kołodyńska, Polym. Adv. Technol. **24** (2013) 866.
3. B. Podkościelna, D. Kołodyńska, Z. Hubicki, B. Gawdzik, A. Bartnicki, Sep. Sci. Technol. **51** (2016) 2501.

Formation of sub- and monolayer nanosystems metal-layered semiconductor

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Self-assembled indium deposition induced nanostuctures formation on the (100) UHV cleaved surface of In_4Se_3 layered semiconductor crystals has been studied by scanning tunneling microscopy/spectroscopy (STM/STS). The STM/STS data were obtained at room temperature with an Omicron NanoTechnology STM/AFM System in UHV better than 10^{-10} Torr. The constant current mode acquisition was used for STM with 400×400 data points resolution. STS was acquired with 80×80 data points resolution. Thermal evaporator EFM-3 was applied for indium deposition *in situ*. Indium ion current inside the effusion cell was maintained to be constant during the indium deposition. The deposition rate was kept at approximately 0.01 ML/min. Small deposition rates were chosen intentionally to produce hetero growth, rather than obtaining of polycrystalline films at high deposition rates. Such rates allow an activation-migration movement of deposited In with localization on growth activation centers.

The study of indium on In_4Se_3(100) substrate sub- and monolayer nanosystems formation was conducted both in "visual" STM mode and in current imaging tunneling spectroscopy (CITS) STS mode. In the last case the matrix of experimental data, so-called, *I-V* curves, spatially acquired over the studied surface area were analysed. Basically, there are well known the different shapes of metal and semiconductor *I-V* curves that depend on value of tunneling current, especially, within bias range corresponding to 0.67 eV energy gap of In_4Se_3. We analyzed the array of studied surface areas with 50×50 nm^2 dimensions to obtain reliable conclusions about metal - semiconductor hetero nano system formation (In/In_4Se_3(100)).

The growth of metallic points quantity on the semiconductor surface depending on indium deposition time that may be powered by consequent thermal annealing conducted after deposition cycle was observed. Both, STM and spatially distributed STS data give evidence that indium deposited nanostuctures' growths has island like, localized nature with next thermal-activated surface migration. Integral STS data over the analyzed area show on formation of indium metal phase on In_4Se_3(100) surface at high deposition times and subsequent annealing.

Physicochemical aspects of behavior of enterosorbents in the gastrointestinal tract

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Active promotion of enterosorbents to the market outruns their thorough study, the mechanisms of their therapeutic effect remain unclear. The general population and even many specialists have a simplified view of the only role of the enterosorbent to fix and remove toxins, that is, act as a "cleaner" of the body. This paper reveals the importance of physicochemical factors for the therapeutic action of enterosorbents. These factors include: (i) electrostatic charge of sorbent's surface; (ii) pore size; (iii) accessable area of surface; (iv) hydrophilic-hydrophobic balance of surface; (v) ability to structurize a water. Mentioned factors can be estimated quantitatively using such methods as electrophoresis, gas chromatography, photon correlation and ^{1}H NMR spectroscopy, *etc*. However, in pharmaceutical practice, it is more convenient to characterize the enterosorbent by the ability to adsorb some test substances. To test the above factors, we use oppositely charged dyes methylene blue and congo red, ions of Zn^{2+}, gelatin, amino acid tryptophan. By the help of this approach we have characterized various types of activated charcoal, nanosized fumed silica (Atoxil), porous Syloid® 244 FP, hydrophobic Aerosil® R972, silica gel, Enterosgel, Smecta®, zeolites, kaolin, some dietary fibers and other materials. To study the impact of enterosorbents on the passage of substances through the mucosa, a gel of vitreous body was used as a model.

We concluded that it is contraversly to classify nanosized silica as enterosorbent, it is rather an enveloping (or mucoadhesive) agent, the main mechanism of action of which is interaction with components of the intestinal mucosa: glycosaminoglycans, glycoproteins, *etc*. As a result, two therapeutic effects are realized: (1) difficulty in diffusion of pathogenic agents through the mucosa and, as a consequence, reduction in their absorption; (2) antidiarrheal effect due to protecting mucosal receptors from the adhesion of microorganisms and impact of microbial toxins. Taking into account that the intestinal mucosa throughout its extent, in the pH range from 6.0 to 8.5, is negatively charged, this interaction for silica occurs with the overcoming of electrostatic repulsion. Therefore, the enveloping power of silica is less than that of aluminum containing Smecta® which in the intestine have a positive charge. Generally speaking, the adsorbing mechanism can only be applied to highly porous sorbents such as activated charcoal, zeolites, silica gel, Syloid® 244 FP: this can be demonstrated by the active extraction of zinc ions from the water solution.

Understanding the concentration distribution in the near-electrode layer in the course of a homogeneous chemical reaction of first order under a model electrocatalytic process

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Theoretical calculation of the concentration distribution of all species in the near-electrode layer in the course of a homogeneous chemical reaction of first order under a model electrocatalytic process on a plane electrode surface was carried out. The role of such parameters of the system as rate constants, diffusion coefficients and equilibrium concentration was determined. The results can be applied for a better understanding of the non-linear behavior at an electrode/electrolyte interface under far-from-equilibrium conditions.

The application of polymeric microspheres with lignin in sorption processes

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Lignin is one of the main constituents in biomass together with cellulose and hemicellulose. It is a complex biopolymer, which contains a large number of functional groups, that is why it shows potential capacities for process of sorption. It is a highly cross-linked polymer with a three-dimentional structure which can provide large surface area and pore volumes [1, 2].

In this work emulsion-suspension copolymerization method, to synthesize the porous microspheres of divinylbenzene (DVB) and lignin was used (Fig.). Before the copolymerization, modification lignin with methacryloyl chloride, to improve its reactivity with other monomers was done [3]. The physico-chemical properties of the obtained microspheres *e.g.* pore structures (adsorption-desorption measurements), thermal properties (DSC), tendencies to swell and the actual shapes were also studied.

Due to well-developed porous structure and the presence of functional groups our materials may have great potential in sorption processes. To estimate the sorption capabilities of the microspheres towards phenol and its chlorinated derivatives the off-line SPE method was applied.

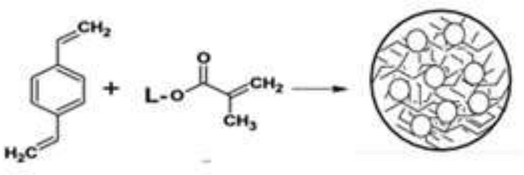

Fig. The scheme of copolymerization

1. M. Canetti, F. Bertini, A. De Chirico, G. Audiso, Polym. Degrad. Stab. **91** (2006) 494.
2. F. Tonin, E. Vignali, E. Pollegioni, P. D’Arrigo, E. Rosini, Enzyme Microb. Tech. **96** (2016) 143.
3. B. Podkościelna, M. Goliszek, O. Sevastyanova, Pure Appl. Chem. **89** (2017) 1365.

Effect of nanosilica-Enoxil composite systems on morphological parameters sprouts tomatoes

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Mineral fertilizers and pesticides, as a rule, pollute the soil with heavy metals and other compounds unusual for it. Therefore, it is necessary to minimize the amount of mineral substances introduced. A promising way to solve this problem is pre-treatment processing of crops seeds with a micro-quantity of composites created on the basis of highly disperse silica and an organic stimulant of plant origin, Enoxil. It is a mixture of polyphenols, esters and carboxylic acids, has stimulating and antimicrobial properties. It can be expected that the silica-Enoxil composite system will ensure the conditions for rapid germination of seeds, their protection from diseases and unfavorable conditions during to the entire growing season.

The aim of this work was a comparative study of the influence composites prepared on the basis of hydrophilic A-300 or hydrophobic AM-1 silica with Enoxil, on the parameters of seed germination of tomatoes.

Ten silica-Enoxyl composite samples were studied in which the Enoxyl concentration was varied in the range of 6-12% by weight. It was shown that the presence of hydrophobic silica (AM-1) in the mixture, for pre-treatment, promotes the growth of the root system of tomato sprouts in all samples, while seed sprouts treated with the A-300-Enoxil composite have a root length less than or equal to the control samples.

In addition, an increase in germination to 97% is observed in samples of seeds treated with the AM-1-Enoxil composite system (with Enoxil concentration of 6, 9, 10% by weight), while seed treatment by analogous composite systems with A-300 shows low germination values (80-92%) close to those in the control sample (87%).

It is interesting, that the increase in the content of Enoxil in the composite to 12.5% by weight leads to a decrease in the value of the germination capacity (85%) of tomato sprouts for both A-300 and AM-1.

The work was carried out with the grant support of the Ministry of Education and Science for the competitive project (No M / 51).

Synthesis and investigation of structural features of silica-supported nickel and cobalt nanocomposite oxides

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In the last decade considerable attention has been paid to the development of novel nanocomposites based on highly dispersed mixed oxide systems. Such composites have wide applicability as adsorbents, catalysts or fillers due to inherent high surface area and the presence of various active surface centres, in particular Brønsted and Lewis acidity, which determine their surface properties. One of the effective methods for synthesis of binary or triple oxide composites is the precipitation of a second oxide phase onto fine disperse silica substrate, in which it is advisable to use fumed silica with non-porous structure. In current work, a series of composites of the composition M_xO_y/SiO_2 (where M are Ni or/and Co) was synthesized. The synthesis was based on solvation-induced adsorption modification of the fumed silica (A300) surface by Ni (II) and Co (II) nitrates with further step-by-step heat treatment up to 600 °C to form the phase structure of the Ni_xO_y, Co_xO_y and Ni_xO_y/Co_xO_y nanooxides. The synthesized samples were analysed by IR spectroscopy, X-ray phase analysis and argon low-temperature adsorption-desorption methods. The structural characteristics of the oxide nanocomposites are shown in the Table. The specific surface area of the synthesized composites is 249-255 m^2/g, which is slightly less than the S_{Ar} of the initial silica (276 m^2/g). According to the results of the XFR, the composites formed NiO crystalline phase and the Co_3O_4 phase with a crystallite size of 14-15 nm (Table), which allows classifying such mixed oxides as nanosized materials. Peaks at 572 and 664 cm^{-1} in the IR-spectrum of Co_xO_y/SiO_2 composites are correspond to Co^{3+} ions vibration in the octahedral hole and Co^{2+} in the tetrahedral hole, respectively.

Table. Structural characteristics of Ni_xO_y, Co_xO_y and Ni_xO_y/Co_xO_y nanooxides

Sample	C_{Ni}, % wt.	C_{Co}, % wt.	S_{Ar}, m^2/g	Oxides phases	$C_{(crystal.phases)}$, %	Average crystal. size, nm
SiO_2	-	-	276	Amorph	-	-
Ni_xO_y/SiO_2	10.5	-	255	NiO	100	15
Co_xO_y/SiO_2	-	10.5	249	Co_3O_4	100	14
$Ni_xO_y/Co_xO_y/SiO_2$	5.25	5.25	251	Co_3O_4 NiO	~64 ~36	14 14

Synthesis and properties of magnetically sensitive nanocomposites based on magnetite and gemcitabine

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The aim of the work is to create new nanotechnologies for chemical modification of the surface of magnet-carrying nanostructures by oncological preparations of the chemotherapeutic and immunotherapeutic mechanism of action, aimed at tumors of hepatocellular carcinoma (HCC) and intrahepatic cholangiocarcinoma (IHCC), synthesis of nanocomposites (NC) containing oncological drug, optimization of physicochemical and technological processes of their obtaining and investigation of physicochemical properties.

Research direction includes synthesis of nanosized one-domain magnetite as a magnetically sensitive carrier, modification of its surface with the aim of stabilization and chemical functionalization, biofunctionalization of NC by immobilization of chemotherapeutic drug gemcitabine (GC).

The processes of adsorption of gemcitabine from its solutions in a physiological liquid on the surface of magnetite and magnetically sensitive NC were studied. Adsorption of gemcitabine is: A = 25-30 mg/g (C_0 = 0.8 mg/mL, g= 30 mg, V = 5 mL). The quantity of GC on the surface of the NC was determined by spectrophotometric method at λ = 268 nm according to the calibration graph.

The magnetic properties of synthesized nanostructures were studied. The synthesized magnet-carrying NC are promising for continuation of the research aimed at the creation of a new nanotechnology for oncology, based on the use of polyfunctional nanostructures capable of recognizing HCC and IHCC tumors, targeted delivery of therapeutic agents of the chemotherapeutic and immunotherapeutic mechanism of action and deposition with additional functions of hyperthermic therapy, and magnetic resonance imaging diagnostics in real time.

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Nanocomposite coatings for protective firefighter uniforms with improved performance characteristics

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It is known that the intensive development of science and technology generates the emergence of increasingly complex emergencies, which are accompanied by fires, including man-made disasters. This circumstance requires more and more sophisticated means of protecting rescuers. Fireman's clothing, as a means of protection, is designed to compensate for the influence of dangerous and harmful factors and contribute to the high and stable performance of the rescuer. Trends and prospects for the development of modern protective clothing were considered in [1]. The conclusion is made about the prospects of creating new types of fibers and polymers, as well as the feasibility of improving existing fire resistant materials due to changes in their structure and surface properties.

This report is devoted to a review of current achievements in the field of obtaining polymer coatings for protective clothing using nanotechnology. New types of coatings based on various polymer binders with the use of inorganic nanoparticles (hydroxides, layered silicates, carbonates, metal oxides) as fillers and flame retardants, as well as methods of their application are considered. Attention is focused on the advantages of nanosized fillers, which consists in their high dispersity (the average size does not exceed 100 nm), which allows to distribute the particles uniformly in the matrix and significantly reduce the concentration of the filler. Textile materials can be given such properties as fire resistance, superhydrophobicity, as well as self-cleaning properties. It is shown that in nanocomposite polymeric materials, nanoparticles interact with the polymer matrix not at the macro level, but at the molecular level. As a result of this interaction, a material is formed that has high adhesion strength of the polymer matrix to the nanoparticle. A method for increasing the fire resistance of textile materials by modifying their surface and obtaining grafted siloxane coatings comprising of phosphorus-containing groups is described. The effectiveness of the use of organosilicon compounds, in particular, AGM-9 monomer, is shown to better combine inorganic oxide nanoparticles with a polymer matrix.

1. E.V. Tarakhno, L.A. Andryushchenko, A.M. Kudin, L.N. Trefilova, Problems of Fire Safety. **36** (2014) 243

Nonadiabatic chemoelectron conversion of the energy of interaction of gas particles with surface

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The dissipation of energy on a surface by means of elementary processes, including electron and phonon excitation, at the instant of the formation of an excited product during an exothermic catalytic reaction is an essential part of physics and chemistry of the surface. An exothermic chemical reaction, as well as the interaction of photons with a surface, leads to electronic excitation of the crystal, provided that most of the chemical energy is converted into electron excitation in a short (femtoseconds) time interval before the adiabatic energy dissipation occurs as a result of the generation of thermal lattice vibrations (picoseconds). Electronic accommodation manifests itself in such phenomena as heterogeneous chemiluminescence (HCL), chemoemission of charged particles from the surface, nonequilibrium chemoconductivity of semiconductors and dielectrics, generation of hot electrons in metals.

The effect of irradiation of wide-gap semiconductors with UV light on the probability of energy accommodation of a heterogeneous chemical reaction (adsorption and recombination of hydrogen atoms) via the electronic channel is studied. It was found that the nonequilibrium electronic channel of accommodation of the reaction energy can influence the rate of the chemical reaction due to the effective transfer of the reaction energy to electrons on shallow electronic traps that are populated by UV irradiation. At the same time, the rate of accommodation of the reaction energy via the electronic channel increases with decreasing energy of the electronic transition in a solid (*i.e.* with decreasing of the depth of the traps).

A micromechanism of transferring vibrational excitation energy to the electronic subsystem of a crystal is considered. The kinetic mechanism of the excitation of a solid by the fluxes of atoms and UV light is built. The probability of accommodation of the energy of a chemical reaction via the electronic channel from the energy of an electronic transition in a solid and the function of the energy distribution of electrons that are generated in the crystal by an exothermic heterogeneous chemical reaction are determined. The efficiency of nonadiabatic chemo-electronic energy conversion in hydrogen power structures based on Schottky nanodiode is calculated.

Preparation, characterization and catalytic activity of nanoceria

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Nanoceria demonstrate high catalytic enzyme mimetic (catalase and superoxide dismutase) activity due to its unique surface structure and the ability of cerium to exist in two oxidation states Ce^{3+} and Ce^{4+}. But it is more stable to the influence of external factors than enzymes. The aim of this work is the preparation of nanoceria, calcination it at different temperatures, the physicochemical properties characterization, experimental determination of it's enzyme mimetic activity in a model reaction of H_2O_2 decomposition.

Nanoceria was synthesised by reaction of cerium nitrate deposition in aqueous medium without stabilizers at room temperature. Nano cerium oxide was heated at 20 °C and calcined in air for 1 hour at 120, 300, 500, 800 °C. The morphology of the synthesised materials was studied by scanning electron microscopy. Sample element content was determined by the energy-dispersive X-ray spectrometry method. The O:C elements ratio in the samples is in the range 1.7-2.1. It is maximal for a sample calcined at 300 °C. XRD method was used to determine the structural characteristics of cerium oxide materials. With increasing annealing temperature, the average size of crystallites and the degree of crystallinity increases. Thus, a sample heated at 20 °C has a degree of crystallinity of 60 % and an average crystallite size of 10 nm, while a sample heated at 800 °C has a degree of crystallinity of 100 % and an average crystallite size of 23 nm. Catalytic activity of nanoceria was studied in the reaction of hydrogen peroxide decomposition at different concentration (1-10 %) at room temperature and within pH 8-11. To determine the kinetic data, volumetric method was used. Catalytic activity of the materials was evaluated using the Michaelis constant (K_m) that was calculated from Lineweaver-Burke plot. The dependence of the nanoceria activity on pH is extreme with maximum at pH 10. The sample calcined at 300 °C demonstrates highest catalytic activity. Water molecules are on the surface of the samples obtained at 20 °C and heated at 120 °C and deactivate catalytic centers. Heating at 300 °C results in the desorption of physically adsorbed water. Catalytic centres are active. Samples calcination at 500-800 °C leads to release from the surface of chemically bound water molecules and to the oxidation of Ce^{3+} to Ce^{4+}. As a result, a decreasing in the catalytic activity takes place.

Complexation of proteins with crown ether-functionalized fullerene?

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We investigated the reactivity without solvents 2-aminomethyl-15-crown-5 (AM15C5), 2-aminomethyl-18-crown-6 (AM18C6), microcrystalline fullerene C_{60}, and the tendency to complexate the resulting compounds with lysozyme in aqueous solutions. The reactions of nucleophilic addition were carried out at temperatures of about 160°C for 5 h. Characterization of the products obtained was performed using Fourier-transform infrared (FTIR) and Raman spectroscopy, LDI-TOF and MALDI-TOF mass spectrometry, scanning electron microscopy (SEM) and thermogravimetric analysis (TGA).

According to TGA measurements, average content of organic fraction in C_{60}-AM15C5 and C_{60}-AM18C6 reaches about 29%. According to the results of SEM imaging and LDI-TOF, macrocyclic reagents are generally unable to deeply penetrate into the bulk of fullerene microcrystals. The resulting complexes are water soluble. MALDI-TOF method shows the formation of a complex between lysozyme and $C_{60}(AM18C6)_3$ in a stoichiometric ratio as 1:1 in water solution.

For additional information on the structure of the functionalized C_{60} complex with lysozyme, we used the molecular docking method. We used the Autodock Vina for computational docking of $C_{60}(AM18C6)_3$ on lysozyme structure. The crystal structure of hen egg-white lysozyme (PDB ID 5WRA), was used as the rigid "receptor" for the docking. As a result, it was identified two binding sites for $C_{60}(AM18C6)_3$, one of which was located in the active site of lysozyme. Predicted binding energies for both these sites ranged between −12.0 and −11.6 kcal/mol.

Methods for description of the textural characteristics of various materials

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There are several ways to describe the textural characteristics of different materials:

(1) adsorption-desorption of low-molecular weight compounds (N_2, CO_2, Ar, C_6H_6, H_2O, *etc*.) in the gaseous (vapor) phase with increasing-decreasing pressure that gives the adsorption-desorption isotherms analyzed in detail using specific software (as well as in the case of other methods);
(2) adsorption of low-molecular weight compounds from liquid solutions with increasing concentration of a solute;
(3) small angle X-ray scattering (SAXS) or small angle neutron scattering (SANS);
(4) quantitative analysis of images recorded using microscopic methods such as HRTEM, SEM, CLSM, *etc*.;
(5) thermoporometry based on DSC or TG measurements with decreasing-increasing temperature;
(6) cryoporometry based on NMR spectroscopy measurements *vs*. temperature;
(7) relaxometry based on NMR spectroscopy and thermally stimulated depolarization current measurements *vs*. temperature.

There are several reasons of the use of these different methods in parallel. For example, a material, which in a native state is strongly hydrated, can change the texture upon drying. Various adsorbates can penetrate in different pores or differently fill pores of different sizes. There are accessible and inaccessible pores (closed or too narrow for used adsorbate), but SAXS can give complete information on all pores in contrast to the adsorption methods.

In this report, application of various methods (see, *e.g*. Fig.) to a variety of materials to describe the textural and structural-adsorption characteristics is described. Additionally, methods of analysis of the experimental data are characterized in detail.

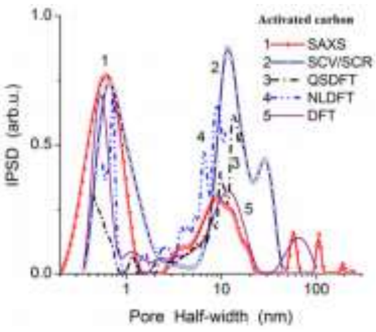

Fig. Pore size distributions for activated carbon (45% burn-off, S_{BET} = 1351 m^2/g, V_p = 1.44 cm^3/g) calculated using SAXS and nitrogen adsorption methods

Effect of structure and chemical state of activated carbon surface on water adsorption

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The investigation of the features and regularities of water vapour adsorption in order to understand the influence of pre-adsorbed water on carbon filter breakthrough performance have an important practical significance. The correlation between adsorption characteristics of three pairs of micro- and mesoporous activated carbons (Norit, NL) towards water and their internal structures defined on the basis of N_2 and CO_2 adsorption isotherms as well as the chemical state of the surface and the nature of primary adsorption sites have been researched in the study. The water adsorption isotherms at low relative pressures have noticeable bulging parts which could be explained by an existence of ultramicroporosity in the carbons or by a significant amount of surface active centers (oxygen functional groups) and the primary water adsorption on them. Features of the pore volume filling for each pair of the activated carbons at average relative pressures (the steep rise of the isotherms occurs at approximately the same p/p_0) indicate the similarity of their microporous structures. The water adsorption capacities for the microporous samples are almost equal (or slightly less) to their micropore volumes determined from nitrogen adsorption isotherms. As opposed to this, a gradual rise of water uptake and the existence of wide hysteresis loops at high relative pressures up to $p/p_0 = 0.95$ are observed for the mesoporous carbons. Moreover, the maximum values of water adsorption in this case considerably exceed the micropore volumes, and are attributable to the capillary condensation in mesopores. The total volumes of water uptake both for micro- and mesoporous activated carbons are significantly less than those determined from nitrogen adsorption. This could be due to a mechanism of cluster pore filling in which the water density is less than its bulk density. Alternatively, it is possible water is not able to condense in the bigger mesopores.

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Evaluation of the sorptive properties of sugarcane bagasse and straw materials for water purification

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One of the promising areas of chemical technology and ecology is the development of new sorption materials based on biomass from annual plants, in particular agricultural wastes. Such an approach will help to solve both the problem of utilization of solid plant wastes and the problem of environmental pollution with organic and inorganic toxicants. Sugar cane bagasse and straw are the agricultural wastes generated in huge amounts annually as by-products of the sugarcane industry. Typically, they are burned with a very low heating efficiency; however, alternative methods for the more efficient use of these lignocellulosic materials are urgently needed. In this study sugarcane bagasse (SCB) and straw (SCS) were used as starting material for preparation of sorbents for metals and dyes. Partial hydrolysis with acetic acid and oxidative delignification with hydrogen peroxide in the medium of acetic acid were performed to modify the sorption properties. The chemical composition, structural and sorption properties of initial and modified materials were investigated.

The adsorption capacity of initial SCB and SCS towards methylene blue was 34 and 37 mg/g, respectively. Treatments of sugarcane biomass allowed increasing sorption capacity of both materials above 50 mg/g. During hydrogen peroxide treatment, the enriching of sorbent with cellulose was observed. In case of pure acetic acid, the formation of lignocellulosic sorbent took place. For sorbents based on SCS, decreased sorption properties towards dyes were observed with the increasing of cellulose content. Inverse dependence in sorption ability was observed in the case of SCB. The same tendency was observed during Fe^{3+} and Cu^{2+} sorption. The results of N_2 adsorption show that all samples based on SCB presented higher values of pore volume in comparison with SCS. SEM method was also used for morphological investigations.

Influence of delignification conditions of solid agricultural wastes on the composition of spent solutions

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The search for new non-waste technologies for the processing of vegetal wastes and by-products of agriculture is carried out in various directions, including biological synthesis of cellulose, enzymatic delignification of wood and solvolytic delignification in the medium of organic solvents. Solvent technologies can be used to develop environmentally friendly pulping processes and allow to utilize hemicelluloses and to obtain reactive lignin from spent solutions with further effective application for different purposes.

The aim of this research work is investigation of composition of spent solutions after solvent delignification of straw with peroxyacetic acid. The increase in the value of the solid to liquor ratio to 9:1 during treatment contributes to reducing the diffusion limitations of the process of transition of delignification products to the pulping solution. The dry residue content of the spent solution reaches 55 kg/m^3, which is obviously the result of the transition the products of the oxidation of lignin, and a significant part of low molecular weight polysaccharides to the solution. The increase in the temperature to 90 °C leads to increasing the the amount of dissolved substances significantly due to the intensification of the process of diffusion from plant material of different extractive substances, lignin, as well as products of oxidation of polysaccharides, and mineral substances. The increase in the concentration of peroxyacetic acid to 10 % also promotes delignification process of initial straw. As a result the amount of dissolved substances reaches 60 %. It was also found out that during straw treatment with peroxyacetic acid from 60 to 120 min, a deep delignification of material takes place, and with further increase in the time of the delignification process up to 180 min the destruction of hemicelluloses and cellulose increases, which adversely affects the chemical composition of the spent solution.

Spent solutions after solvent delignification of straw can be used for further conversion into sugar and alcohols, also a low molecular weight lignin can be obtained by precipitation.

Metal decorated graphene as novel electrocatalyst for solid acid fuel cells

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Fuel cells (FCs) convert chemical energy directly into electrical energy with high efficiency, high power density and virtually zero emission of pollutants. Despite tremendous efforts, developing electrocatalysts used in FCs with high activity at low cost remains a great challenge and a critical limitation to their large-scale commercialization. The hybrid materials based on metal and metal oxide nanoparticles supported on carbon materials have received a great deal of attention owing to their wide range of potential applications in electrochemical conversion, energy storage devices and solar cells. This study focuses on the molecular and electronic structure of graphene/platinum decorated graphene to enhance the long-term durability of Pt nanoparticle electrocatalysts and highlight solutions to improve the electrical conductivity, surface shape and the strong interaction between the nanoparticles and the supporter for fuel cell applications.

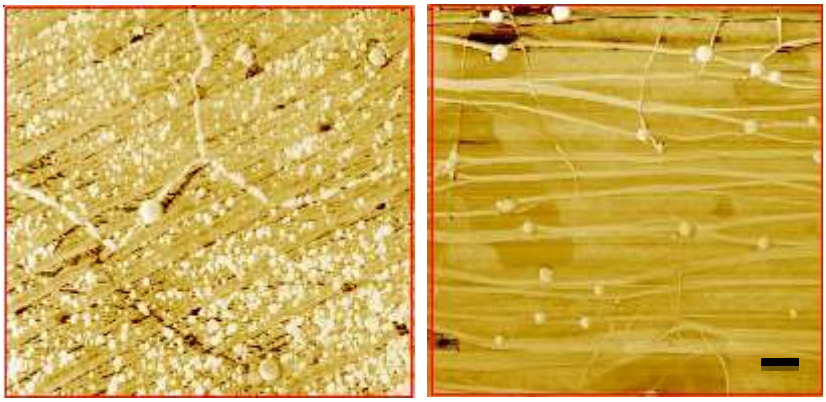

Fig. AFM for graphene (right) and Platinum nanoparticles on Graphene (left), scale = 200 nm

Interaction of visible electromagnetic radiation with periodic nanostructures

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Thanks uniquely combined optical and electrical characteristics, Si nanowires (SiNWs) have received considerable attention for solar cell application. These structures have been shown to have enhanced absorption compared with thin films, however the mechanism responsible for this is not understood [1].

In nanowired solar cell applications SiNW arrays vertically aligned to the substrate demonstrate broadband optical absorption due to strong light trapping by multiple scattering of the incident light. Since the typical geometric factors of SiNWs, including wire diameter, length, and periodicity, are known to significantly affect the optical properties, a costefficient, optimized technique is critically needed to precisely control the major dimensional variables for solar cell applications [2].

Using numerical method FDTD (Finite-Difference Time-Domain) was calculated distribution of the electric and magnetic fields on the surface of the structure with nanowires. The nanowires have the following dimensions: height – 2330 nm, diameter – 80 nm, period – 100 nm (Fig. 1). It is shown that the distribution of the electric field is concentrated in the air gap between the nanowires (Fig. 2), in contrast to the magnetic distribution, which is concentrated on the nanowires themselves.

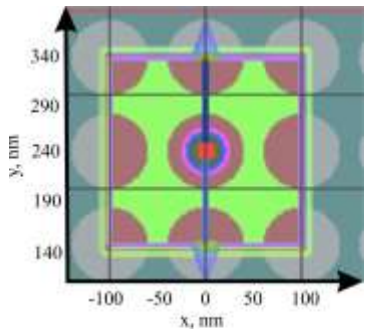

Fig. 1. Schematic image of the calculated area

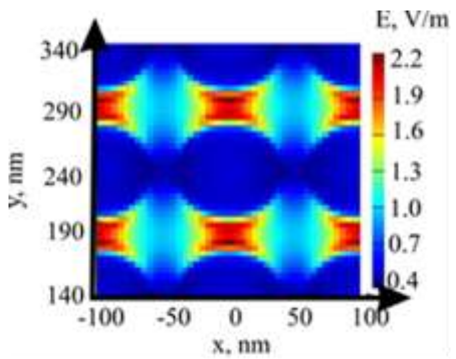

Fig. 2. Field distributions of the dominant transverse electric field component at the absorption peak wavelength of 500nm

1. J. Li, H.Yu. Yu, S. M. Wong, X. Li, G. Zhang, P. Guo-Qiang Lo, D.-L. Kwong, Applied Physics Letters. **95** (2009) 243113.
2. J.-Y. Jung, Z. Guo, S.-W. Jee, H.-D. Um, K.-T. Park, J.-H. Lee, Optics Express. **18**(S3) (2010) A286.

Genesis of surface films as a self-organized criticality: Computer model

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On progress of physical methods for controlling the structure of thin films on the surface of solids in the process of their formation, a computer model of a film as a percolation system with self-organization was proposed.

Percolation problems with self-organization form an integral part of the theory of self-organizing criticality, which was proposed in [1], first of all, to comprehend the connection between the local structure organization and the mechanism of criticality development [2]. The most general patterns of the evolution of percolation systems with interacting elements include the existence in them of nonequilibrium quasistationary states, arising due to multiscale correlations in space and time [3].

The construction of the cluster system in the model is carried out by the Monte Carlo method using an iterative algorithm for realizing the interaction of its elements and two variants of the law of attraction: with forces proportional to $1/R^2$ or $1/R$.

The dependence of the structure and properties of self-organizing clusters on the degree of self-organization, characteristic values of the correlation length, generation rate of the system has been investigated in the model. For that in the model studied their dependence, respectively, on the number of acts of particle interaction, on the maximum distance at which elements of the system can be combined into a cluster, as well as on the number of particles generated at the percolation field at each step of creating an infinite cluster.

Analytical expressions are obtained for the dependence on these parameters of the power of an infinite cluster, its radius of gyration, degree of anisotropy, and lacunarity; the fractal and first two correlation dimensions of the Renyi spectrum are also calculated in the research.

1. P. Bak, C. Tang, K. Wiesenfeld, Phys. Rev. A. **38** (1988) 364.
2. A. Herega, Nanomechanics Science and Technology. **4** (2) (2013) 119.
3. L. Zelenyi, A. Milovanov, Phys. Usp. **47** (2004) 749.

Sorption and mechanical properties of POSS-containing nanocomposites based on PU/PHPMA semi-IPNs

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The nanocomposites based on semi-interpenetrating polymer networks (sIPNs) consisting of the crosslinked polyurethane (PU) and linear poly(hydroxypropyl methacrylate) (PHPMA) in relation to PU/PHPMA=70/30, and with 1,2-propandiolisobutyl-POSS as nanofiller (1-10 wt%) were created. The effect induced by the POSS incorporation on sorption and mechanical behaviour of the nanocomposites has been investigated.

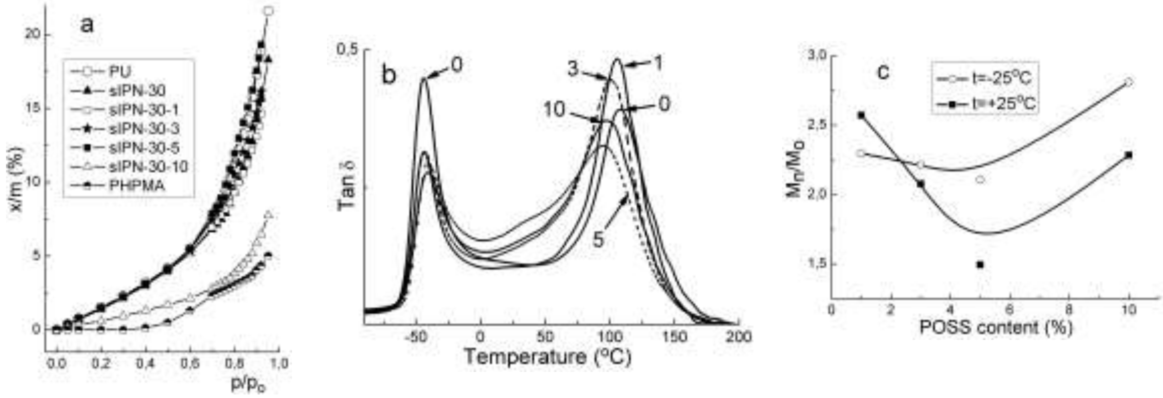

Fig. The isotherms of dichloromethane (DCM) vapours sorption (*a*), the temperature dependences of the loss factor (tan *δ*) (*b*), and the relation of the nanocomposite's storage modulus to matrix's modulus Mn/Mo versus POSS content at different temperatures: +25°C and −25°C (*c*); *x/m* is the amount of DCM relative to the dry sample; p/p_0 is the relative pressure of DCM

From Fig. *a* evident that the values of vapour sorption by nanocomposites are less in compare with native matrix semi-IPN-30 for all concentrations of POSS in the samples.That means the formation of more dense structure of the nanocomposites in compare with matrix semi-IPN-30 occurs.

Fig. *b* shows two peaks of Tan δ, thus all semi-IPN-30 nanocomposites are two-phase systems with incomplete phase separation. The glass transition temperature of the second PHPMA peak in the semi-IPN-30 is shifted towards low temperatures with increasing the POSS content.

The storage moduli of the nanocomposites based on semi-IPN-30 (Fig. *c*) exceed the storage modulus of the native matrix and they change in nonmonotonic way with POSS nanofiller content. In this case nanofiller affects the second component of matrix – PHPMA, as result the reinforcing effect of the semi-IPN-30 nanocomposites occurs.

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Sorption of noble metals on surface silica gel and phytosorbents with chemical grafted thiourea groups

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Extraction and determination of the noble metals (NM) microamounts from industrial solutions is a pressing challenge. For this goal, the new sorbents with chemical grafted thiourea groups based on aminopropylsilica gel (TSS) and crystalline cellulose and pine (phytosorbents) were synthesized. Synthesis of sorbents was carried out on the following reactions:

$$[\text{Si-O-Si}](CH_2)_3NH_2 + NH_4SCN = [\text{Si-O-Si}](CH_2)_3NH(CS)NH \text{ (TSS)}$$

$$\text{R-OH} + NH_4SCN = \text{R-NH(CS)NH, R- molecule cellulose or pine (phytosorbents)}$$

These processes have been studied by thermogravimetry / differential scanning calorimetry (TGA/DSC), scanning electron microscopy (SEM), and Fourier transform infrared spectroscopy (FT-IR). A specific surface area and pore volume of synthesized sorbents was investigated.

The maximum degree of NM extraction by investigated sorbents is achieved in a medium of 1 M HCl - pH 3. The time to achieve the sorption equilibrium does not exceed 15 min (TSS) and 24 h (phytosorbents), which is due to diffusion processes with NM sorption. When heated, the sorption equilibrium is achieved in an hour. The sorption capacity in TSS is, mmol/g: 0.75 for Pd(II), 0.075 for Au(III) and 0.065 for Pt(IV). The sorption capacity on phytosorbents is much higher than the sorption capacity on silica gel and is 1.2 mmol/g for Pd(II), 0.3 mmol/g for Au(III) and 0.75 mmol/g for Pt(IV), which is due to different concentrations of grafted thiourea groups and their arrangement in the volume of sorbents.

The sorption-colorimetric method of NM determination on the surface of TSS, the core of which is the ability of the NM to form colored complexes with thiourea has been developed. The possibility of using phytosorbents for the extraction of NM from industrial solutions with the subsequent combustion of the sorbent and get metal powder or metal desorption by thiourea solution for the production of these metals concentrates is considered.

The effect of substrate bias on structure, optical and electrical properties of wide bandgap oxides films

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The wide bandgap *n*- and *p*-type semiconductor oxides (E_g=3.3–4.0 eV at room temperature) have attracted considerable attention due to their great potential application in such transparent electronic (TE) fields as display technology, ultraviolet optoelectronics and solar cells. *n*-ZnO (E_g=3.3 eV) and *p*-NiO (E_g=3.4 eV) are wide bandgap oxides which are interesting materials for designing TE devices due to its elemental abundance, large direct band gap and many available deposition technologies. Therefore, the development of technology for deposition of quality *n*-ZnO and *p*-NiO films is very important and actual task of present materials science.

Reactive magnetron sputtering (MS) is believed to be most widely used growth method due to good films adhesion, high deposition rates, films uniformity of over large areas of the substrates and flexible control over the composition of the deposited films. It is clear that the improvement both crystal quality of *n*-ZnO and *p*-NiO films and their optical and electrical properties can be reached by the step-by-step optimization of deposition parameters. To our best knowledge, the influence of bias voltages applied to substrate (substrate bias) on the structure, optical and electrical properties of *n*-ZnO, *n*-ZnO:Al and *p*-NiO has not been studied yet.

Our report devoted to investigation of the influence of substrate bias on structure, optical and electrical properties of ZnO, ZnO:Al and NiO thin films deposited on Si and glass wafers by using layer-by-layer growth method at MS [1]. X-ray diffraction, Raman scattering, photoluminescence, Fourier transform infrared spectrometry, optical transmission and electrical measurements were used for samples characterization. It was found that the application of bias voltages to wafer allow us to sufficiently influence on the properties of widegap oxide films. Obtained results will be analyzed and discussed.

1. A.I. Ievtushenko, V.A. Karpyna, V.I. Lazorenko, G.V. Lashkarev, V.D. Khranovskyy, V.A. Baturin, O.Y. Karpenko, M.M. Lunika, K.A. Avramenko, V.V. Strelchuk, O.M. Kutsay, Thin Solid Films, **518**, (2010) 4529.

Monitoring of structural and surface properties of platinum ions doped titania films with different surface morphology

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Platinum supported catalysts have been used for different reactions: chemical synthesis, environmental catalysis and fuel conversions. The unique catalytic properties of platinum prompted the investigation of Pt modified titania for photocatalytic applications as well. Pt doped titania systems are perspective in the way of the solar light application in ecological photocatalysis. Platinum in titania matrix allows to absorb the light with lower energy, stimulated the adsorption of the gaseous or liquid pollutant molecules and acts as a charge trapping centre. However, its oxidation state is one of the crucial factors during catalytic or photocatalytic transformations.

The sol-gel approaches of mesoporous and nonporous titania doped with platinum ions in the form of the thin films are presented. A three-block copolymer Pluronic P123 as a template and acetylacetone as a stabilizing agent have been used to create the mesoporous structure of the films. The nonporous films are formed using the simpler and faster route based on the hydrolysis of titanium(IV) isopropoxide in ethanol medium. The use of platinum(II) acetylacetonate in conjunction with the different pretreatments is suggested to cause the formation of platinum in its different valence states within titania matrix. The presence of acetylacetonate as a counter ion can stimulate the incorporation of the doping agent during sol ripening.

As revealed by XRD analysis, the crystallization of titania to anatase and mixture of anatase/brookite was observed for 1%Pt/TiO_2 films synthesized without (nonporous) and with template (mesoporous), respectively, pointing on the influence of the synthesis procedure on the crystallization rate of titania. The ratio of the elements into the film bulk is calculated by means EDS data. Homogeneous distribution of the elements is proven by EDS mapping images. As shown by XPS analysis, the partial reduction of Pt(II) to Pt(0) takes place under synthesis conditions of mesoporous structures. In opposite, two oxidation states of platinum ions, as namely Pt^{2+} and Pt^{4+}, are registered by XPS onto the surface of nonporous films. The Pt : Ti ratio in the film surface is varied depending also on the synthesis procedure. Thus, the required film composition can be achieved selecting the certain synthesis conditions.

Effect of physicochemical actions on surface properties of diamond nanopowders

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Nanopowders of detonation synthesis diamond (DSUD) of various modifications are manufactured in many countries. The study and formation of the characteristics on which the effectiveness of the application of DSUD depends is the actual task for the creation of new materials.

The purpose of this work is the development of physical and chemical basis for the formation of surface properties of DSUD.

DSUD investigations were carried out by scanning electron microscopy and physico-chemical methods.

It is established that changes in aggregative, electrophysical, adsorption-structural characteristics, hydrophilic-hydrophobic balance of the surface, degree of chemical homogeneity of surface occur as a result of surface reconstruction, i.e. changes in its structural and chemical composition.

For example, the two-stage gas-phase thermal treatment of the powder allows to increase the porosity by 1.8 times, the specific surface area and adsorption activity to metal ions, to saturate the functional coating with oxygen-containing groups and to reduce the area of conducting centers; freezing leads to the ousting of oxygen-containing groups, aggregation of aggregates 7-fold, and an increase in physico-mechanical characteristics. Reduction in the rate of aggregation and disaggregation of particles occurs as a result of the dissociation of surface oxygen-containing compounds and a change in the surface charge. A criterion (K) is proposed that characterizes the chemical homogeneity of the surface, which is equal to the fraction of the specific surface area of the DSUD, which is occupied by current-carrying centers. The smaller the value of K, the more uniform the surface. As a result of two-stage gas-phase heat treatment K=3%, electrochemical reduction treatment K = 3.8%, electrochemical oxidative treatment, thermo-chemical treatment K = 2.8%.

Fractionation of DSUD with a reconstructed surface by sedimentation under dynamic conditions; in a magnetic field, the adhesion-magnetic method makes it possible to increase the uniformity of powders in 1.6-2.1 and 1.2-1.3 times, respectively.

Ion-exchange and bactericidal properties of oxidized carbons with adsorbed ions of silver, copper and zinc

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Development of new bactericides with adsorbed ions of Ag^+, Cu^{2+} and Zn^{2+} on different carriers is a topical problem of modern material science. Recently, it has been proved that active component of bactericidal materials is precisely the ions of these metals, not their nanoclusters or coarse phases. We propose oxidized activated carbon “Chemviron Carbon” (Belgium) as carrier for adsorbed ions. This technical carbon is inexpensive and has well-developed and adjustable porous structure. Carbon samples with a bulk density of 0.34 g/cm^3, specific surface area of 1740 m^2/g and pore volume of 0.814 cm^3/g were used in the experiments. Sorption of silver, copper and zinc ions was carried out at room temperature for 24 hours. Bactericidal properties of obtained materials were studied against *Pseudomonas aeruginosa* and *E. coli*.

It turned out that bactericidal activity of oxidized carbon with a small amount of adsorbed silver ions (0.01-0.1% by weight) mainly surpassed that of activated carbon with metal nanoclusters or its coarse phases in amounts of 1-3% by weight. The results of microbiological analysis are supported by the SEM data which demonstrate amount of metallic phase on the surface of activated and oxidized carbon. Samples of oxidized carbon with significantly smaller amount of reduced metal exhibited greater bactericidal activity.

Activity of synthesized materials increases with a raise of oxidation degree of carbon surface. We studied the samples which had static exchange capacity (SEC) of 0.2; 0.6; 1.6 and 2.3 mg-eq/g. Activity increase is due to SEC increase, in connection with which part of adsorbed silver in the form of Ag^+ ions increases and part of Ag^+ ions reduced on unoxidized sections of carbon surface decreases. Comparative study of bactericidal activity of silver, copper and zinc ions was also conducted. It was established that activity of Cu^{2+} and Zn^{2+} adsorbed on carbon yielded to Ag^+ in 20-30 and 50-60 times, respectively.

Oxidized “Chemviron Carbon” with adsorbed Ag^+ (0.01% by weight) or mixture of Ag^+ and Cu^{2+} (by 0.05% by weight) showed high bactericidal action against *E. coli*. The microbiological analysis was conducted in a static mode. It was found that desorbed ions provided for inhibition of bacteria growth and their destruction in suspension around the samples. These results make it possible to use obtained materials as active components of bactericidal dressings for treatment of infected wounds, trophic skin lesions, ulcers, burns, *etc*., as well as for treatment and disinfection of drinking water.

The high-energy nanoreactors in condensed matter

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In this paper we consider high-energy phenomena at the nanometer level, which are generated by self-consistent molecular fields acting on individual particles [1, 2]. The analysys is carried out using the Bogolyubov-Born-Green-Kirkwood-Yvon equations for the particle group distribution functions. A number of such phenomena include: 1) the emission of atoms, molecules with superheating rates from the open surface of a condensed system; 2) implosion of the convergent streams of high-energy particles, accompanied by the phenomena of their shock dissociation and ionization with the formation of partially ionized plasma; 3) the recombination of plasma ions and electrons and the formation of molecules with the release of significant kinetic energies. As examples, being considered the molecular-kinetic mechanisms of such mysterious phenomena as sonoluminescence in liquids, phenomena of detonation in condensed systems, initiation of earthquakes with rapid opening of faults and others are considered.

The nature of all such phenomena is based on the action of high-energy self-consistent multiparticle forces on a nanometer scale, which are defined as nanoreactors. In nanoreactors, the evolution of condensed system composition is governed by balance transition between the potential energy of the system and the kinetic energy of the particles. The most important consequence of the series of microscopic high-energy phenomena is a possibility of emission from an open surface of condensed systems of atoms and molecules with significant superthermal velocities. Under certain thermodynamic conditions, the workfunction of the atoms and molecules from the surface of the system can take negative values [1, 2]. The phenomenon of high-energy emissions due to the balance of the impulse has a property of self-amplification and leads to a generation of shock waves of rarefaction. The phenomenon of implosion of emitted streams, which is accompanied by shock dissociation and ionization, occurs in cases of rapid opening of pores or cracks. Recombination in incompletely ionized plasma causes the allocation of thermal energy and resulting thermal explosions.

1. S.D. Kaim, Nanophysics of high-energy phenomena in condensed matter, VMV: Odesa, 2011.
2. S.D. Kaim, Statistical theory and modelling of high-energy phenomena in tectonophysics, VMV: Odesa, 2015.

Synthesis and properties of nano-structured silica modified by nitrogen-containing compounds

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The most common way of creating functionalized silica composites is to obtain a carrier - amorphous silica with its subsequent modification. Of particular interest are SiO_2 sorbents with fixed nitrogen-containing compounds that detect complexing, ion exchanging properties and, according to scientific assessments, are sufficiently effective in extracting and further defining some heavy metal ions, oil products, as carriers of drugs; on their basis create modern sensory systems. However, the synthesis process is usually complex, multi-stage, requires the use of complex organosilicon precursors and maintain certain temperatures and pressures. Accordingly, the creation of effective silicic sorbents based on simple and accessible materials and technologies is currently relevant.

We conducted colloid-chemical synthesis of nano-silica minerals, modified using the precursors - soluble glass and diphenylamine (DFA). The modification was carried out under conditions in which the DFA during the formation of the silica nanoparticles can oxidize, dimerize, form oligomer compounds and, at the same time, be fixed in the structure of SiO_2 - cluster or aggregate. The modification occurs in the process of dynamic growth of a spherical silicone nanoparticle and continues with further association and aggregation of particles with the formation of hydrogel. In this synthesis, nano-silica was used as a matrix in the structure of which the layers of organic matter bound to the surface of a solid formed. To limit the uncontrolled increase in growth and the simultaneous «loosening» of silica particles, a polydyphenylsilanediol was added to the reaction system.

The physicochemical properties of modified silica were studied by methods of nitrogen adsorption and IR spectroscopy.

The analysis of the obtained materials showed that the synthesized silica is mesoporous, they have been modified with nitrogen-containing compounds, in particular N,N-diphenylbenzidine, and by the magnitude of the specific surface area and the specific pore volume, they are not inferior to the properties of known SiO_2-based sorbents that are currently used in medicine and ecotechnology.

Rice husk – bio-renewable sources for the obtaining of amorphous silicon dioxide and carbide for manufacturing different materials

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The wide use of inorganic silicon compounds, such as silicon dioxide and silicon carbide, in various industries, still leaves open the question of creating an efficient technology for the production of the above-mentioned ultra-pure materials. Rice husk is one of the promising sources of bio-silicon-containing compounds. It's a waste of agricultural activities. About 75 thousand tons rice husk are formed in Ukraine every year.

The use of fluoride-salt technology allowed extracting silica from the fly ash part of husk with 100% yield. The purity of the obtained material is 99.9995% that was established by ICP method. Silicon dioxide is in the amorphous state that was confirmed by X-ray diffraction analysis and formed the 200-300 nm spherical agglomerates (Fig. 1). The specific surface area of the material is 105 m^2/g.

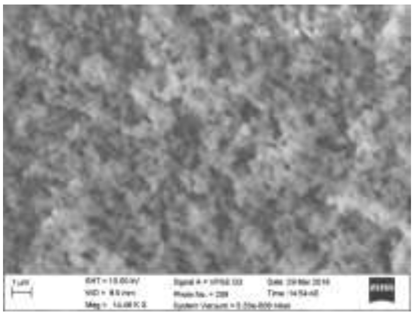

Fig. 1. SEM images of amorphous silicon dioxide

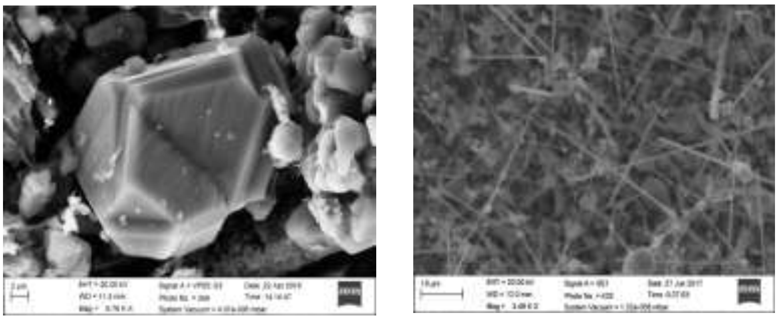

Fig. 2.SEM images of silicon carbide

The direct production of silicon carbide from rice husk was developed. It consists of high-temperature treatment of the raw materials and follows purification of the desired product from impurities. Using X-ray phase analysis it was established that silicon carbide synthesized by this technology has a cubic structure. The purity of the material is 99.9998%. Fig. 2 shows the possibility of producing silicon carbide in the form of particles or fibres.

The theory of photomotors: stochastic processes with deterministically changing transition rates

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Brownian photomotors are the systems which can move directionally when rectify light-induced nonequilibrium fluctuations. In photomotors [1], the time dependence of a particle potential energy is induced by cyclic laser pulses resonant with certain levels of its electronic subsystem. There are plenty of nanomachines producing directed motion, rotational or translational, under the action of light-induced unbiased perturbations [2,3].

We study Brownian photomotors governed by stochastic processes with deterministic dichotomous changes in transition rates. The kinetics of a 3-level system with arbitrary rate constants of transitions between the levels is considered; the rates are different depending on the intensity of a laser pulse. The mathematical model is a system of differential equations for the populations of electronic levels, $n_j(t)$, $j=1,2,3$. With $n_j(t)$, one can calculate the particle charge distribution $P(\mathbf{r},t)$ and potential energy $U(\mathbf{r},t)=\iiint_V d\mathbf{r}'P(\mathbf{r}',t)\varphi(\mathbf{r}+\mathbf{r}')$ of its interaction with a polar substrate (a source of the electrostatic potential, $\varphi(\mathbf{r})$). This system can be treated as a particular case of the Pauli equation, for a stochastic Markov process of transitions between N (with $N=3$) states, for the conditional probability $\rho_{nn'}(t)$ to find the system in a state n at time t, if it was in a state n' at time $t=0$: $d\rho_{nn'}(t)/dt+\sum_{n''}\Gamma_{nn''}(t)\rho_{n''n'}(t)=0$, $\rho_{nn'}(0)=\delta_{nn'}$. The matrix Γ is time dependent; it is different for time intervals τ_+ and τ_- with the laser turned on and off, and thus is described as a deterministic dichotomous process: $\Gamma_{nn''}(t)=\Gamma_{nn''}^{(+)}$ for $r\tau<t<r\tau+\tau_+$ and $\Gamma_{nn''}(t)=\Gamma_{nn''}^{(-)}$ for $r\tau+\tau_+<t<(r+1)\tau$, $r=0,1,...$; $\tau=\tau_+ +\tau_-$ is the period of the cyclic process. This model is analyzed analytically and numerically. The redistribution of the populations, $n_j(t)$, with time under the cyclic laser pumping is demonstrated, as well as the changes in photomotor potential energy as a result of it. The conditions under which the maximum photomotor velocity is reached is analyzed. The results are discussed in the context of a Brownian photomotor based on a semiconductor nanocluster [1].

1. V.M. Rozenbaum, M.L. Dekhtyar, S.H.Lin *et al.*, J. Chem. Phys. **145** (2016) 0641101.
2. M.L. Dekhtyar, A.A. Ishchenko, V.M. Rozenbaum, J. Phys. Chem. B. **110** (2006) 20111.
3. J. Michl, E.C.H. Sykes, ACS NANO. **3** (2009) 1042.

Sorption of dichromate anions on mesoporous silica functionalized with aminopropyl groups

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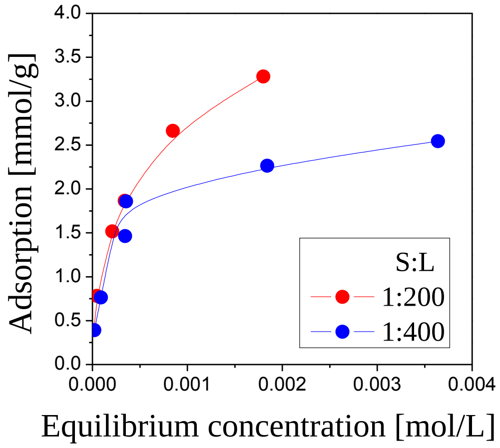
Chromium is a toxic element, dangerous pollutant, sources of which are sewage sludge of tanneries, discharges and emissions of metallurgical enterprises. The maximum contaminant level standards, for Cr(VI), established by United States Environmental Protection Agency is 0.05 mg/L. Presumably, materials with a high specific surface area and a uniform dense layer of Lewis acids on it can provide high sorption parameters for the extraction of chromates. Ammonium groups refer to Lewis acids. A sample SBA-15/NH_3^+ was synthesized according to [1]. The influence of the solid-liquid ratio on the adsorption of dichromate was investigated for this sample (Fig.). The distribution coefficient and the sorption capacity are shown in Fig.



	1:200	1:400
Langmuir model:		
Kd, cm^3/g	15643	12807
Kex	4343	4833
Emax, mmol/g	3.60	2.65
R^2	0.98315	0.9963
Freundlich model:		
K_F	62.1	24.1
1/n	0.45	0.37
R^2	0.98	0.90

Fig. $K_2Cr_2O_7$ sorption isotherms for various solid-liquid ratios

The sample contains 0.55 mmol/g of ammonium groups. The ratio of dichromate anions to ammonium groups is 6.55 at solid-liquid ratio 1:200 and 4.82 at 1:400. That may indicate the formation of polychromates on the surface of this sample.

1. V.V. Sliesarenko, O.A. Dudarko, Yu.L. Zub *et al.*, J. Porous Mater. **20** (2013) 1315.

Effect of substitution of magnesium ions on the structure and morphology of nanoscale lithium ferrite

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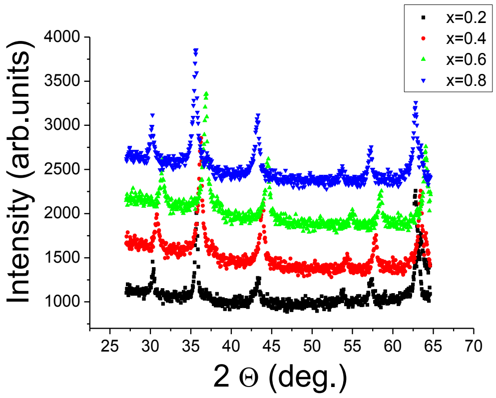

Fig. Experimental X-ray diffraction patterns of systems $Li_{0.5}Fe_{2,5-x}Mg_xO_4$ (x=0.2; 0.4; 0.6; 0.8)

Nano sized magnesium-substituted lithium ferrites of the total composition $Li_{0.5}Fe_{2,5-x}Mg_xO_4$ (x=0.2; 0.4; 0.6; 0.8) were obtained by sol-gel self-combustion with a metal / fuel ratio of 1:1.75 and a neutral reaction medium (pH = 7).

Figure shows experimental X-ray diffraction patterns of samples synthesized by the sol-gel self-combustion method, with different content of magnesium ions.

All systems are single-phase spinels of the spatial group Fd3m. The main structural and morphological parameters of the synthesized systems are given in the table

Table. Structural and morphological parameters of nanosized magnesium-substituted lithium ferrites

The content of magnesium ions x	X-ray density d_x, g/m^3	Picnometric density ρ, g/m^3	Dimensions of crystallites *D*, nm	Molar mass *M*, g/mole	Relative porosity *P*, %	Active surface area *S*, m^2/g
0.2	4.64	2.13	17	200.70	0.54	168
0.4	4.46	2.42	21	194.46	0.46	116
0.6	4.29	1.99	15	188.16	0.54	200
0.8	4.16	1.56	14	181.85	0.63	268

The average size of crystallites of synthesized samples is in the vicinity of 14 - 21 nm, and the surface area calculated on the basis of the ratio $S=6000/(D\rho)$ is 116-268 m^2/g, which indicates the nanocrystalline nature of the samples obtained.

Effect of bile salts on adsorption of cholesterol on hydrophilic/hydrophobic silica surface

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Hypercholesterolemia is associated to an abnormal increment of cholesterol in the blood. This excessive cholesterol can cause heart attacks, atherosclerosis, hypertension, vascular brain illness as well as gallstone formation. Such cholesterol concentrations can be diminished by eating a low cholesterol diet or exercising; but sometimes this strategy is not enough to decrease cholesterol levels. The possibility of the excretion of excess cholesterol from an organism by adsorption is of great interest.

It is known that bile salts solubilize cholesterol due to the formation of mixed micelles. Therefore, the adsorption of cholesterol and several bile salts (taurocholic, cholic, deoxycholic, and chenodeoxycholic) on the surface of partially hydrophobized by trimethylsilyl groups silica adsorbent from individual and mixed solutions was studied at constant solution pH 7.4 as a function of the concentration of bile salts. The PM7 method and the COSMO solvation model implemented in the MOPAC2016 software package were used to determine the adsorption mechanism.

The values of Gibbs free energies of adsorption (PM7) such as the experimental values of bile salts adsorption correlate with partition coefficients in the *n*-octanol–water system, which characterize the hydrophobicity of bile salt molecules. The experimental and quantum chemical results demonstrate that cholesterol is adsorbed on the surface of silica adsorbent as an individual compound, even from solutions, in which it is solubilized due to interaction with primary micelles of bile salts. Apparently, the part of cholesterol is released from micelles and adsorbed on the silica surface. The stronger the bonding of cholesterol with bile salt micelles, the smaller its adsorption on the surface of adsorbent.

Effects of ultrasonic impact treatment on physical and chemical state of the surface layer of Zr1Nb alloy

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To date, the required level of physical and mechanical properties of the newest materials can be achieved owing to the formation of ultrafine-grained (UFG) and nanocrystalline (NC) grain structures. One of the most effective methods of the grain subdivision in the surface layers of metallic materials is ultrasonic impact treatment (UIT). The mechanism of the formation of UFG microstructures and experimental evidence regarding their beneficial effect on the corrosion resistance was described in [1, 2]. The factors contributing to the formation of UFG and NC microstructures were concluded to be the following: high frequency of shock impulses, the presence of a shear component of deformation during impact, local heating of the surface layers during UIT-induced severe plastic deformation.

This study presents new results of the EDX, SEM and XRD analyses of the oxygen content in the cross-section of the UIT-processed Zr-1% Nb alloy. It is shown that the oxide film t-ZrO_2 with tetragonal structure is formed, which is more dense, stable and corrosion-resistant as compared to the monoclinic m-ZrO_2 oxide.

Saturation of the surface layer with oxygen is an additional strengthening factor of the alloy owing to at least two factors. Firstly, high oxygen content (up to 30%) promotes the formation of an interstitial solid solution of oxygen in zirconium, and, secondly, the oxide film is formed.

Understanding of the correlation relationships of structural changes and phase transformations under multiple impact loads and anticorrosion properties of the surface layers of zirconium alloys is an urgent task. Additionally to a good biocompatibility of zirconium, the application of ultrasonic impact treatment allows further enhancing corrosion resistance and mechanical properties by low-temperature oxygenizing by the strain-induced mechano-chemical reactions.

1. B.N. Mordyuk, O.P. Karasevskaya, G.I. Prokopenko, N.I. Khripta, Surf. Coat. Technol. **210** (2012) 54.
2. B.N. Mordyuk, O.P. Karasevskaya, N.I. Khripta, G.I. Prokopenko, M.A. Vasylyev, Metallofiz. Noveishie Tekhnol. **36**, № 7 (2014) 917.

Destruction of hydrocarbons by composite system based on the nanosilicas and yeast cells mixture in aqueous medium

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The problem of water and land purification from oil products pollution by becomes more and more relevant every year. Nowadays, the most promising method is bioremediation based on the oxidation of petroleum products by microorganisms (bacteria and fungi) which are capable to destroy hydrocarbon compounds to ecologically harmless substances due to the consumption of oil products as a source of their vital energy. Therefore, the aim of this study was to determine the effect of the mixture hydrophilic (A-300) and hydrophobic (AM1-300) nanosilicas on the vital activity of *Saccharomyces cerevisiae* yeast cells using as a biodestruction agent of motor oil in the aqueous medium.

It has been found that as part of the nanocomposite the optimal ratio of A-300:AM1-300 is 1:1 with the yeasts amount of 50%. An increase in the amount of hydrophobic nanosilica over 50% leads to not wetting by water of this nanocomposite and a sharp decrease in the number of cells interacting with silica.

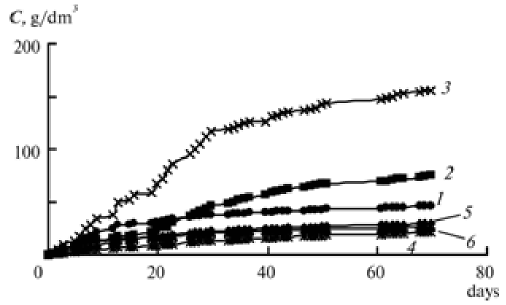

Fig. Kinetic curves of the carbon dioxide release from the *S.cerevisiae* suspension in nanocomposite with weight 0.1 (*1*), 0.5 (*2*) and 1.0 g (*3*) in comparison with the control samples containing 0.05 (*4*), 0.25 (*5*) and 0.50 g (*6*) of pure yeast in the nanocomposite

The hydrophilic and hydrophobic nanosilicas as part of the composite system promotes the activation of the vital processes of cells by 2.5 times at a solid phase concentration $C_s = 0.5$ g and almost 6 times at $C_s = 1$ g, in comparison with the control. The amount of CO_2 by suspension of cells emission increases almost in twice with the increase in the nanocomposite concentration. Thus, studied nanocomposite is an effective biodestruction agent of motor oil hydrocarbons in the aqueous medium.

Adsorption of surfactants mixtures from aqueous solutions by carbon sorbents

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The studying of mutual interactions of nonionic surfactants during adsorption on solid surfaces is very important to provide a better insight into different colloid-chemical processes and to predict the properties of surfactants mixtures. In this work adsorption of nonionic and anionic surfactants from their binary aqueous solutions and at different surfactants content on the surface of graphitized black carbon was investigated.

Sodium hexadecyl sulfate (HDS) and oxyethylated octylphenol Triton X-100 with an oxyethylation degree of 9-10 (TX-100) were used as anionic and nonionic surfactants, respectively.The specific surface area of the graphitized carbon black evaluated by BET method with argon adsorption was 105 m^2/g. Mixed HDS - TX-100 systems have been studied over a concentration range of (1.5-5.0) 10^{-5} mol/dm^3. The molar fraction (n) of TX-100 in the solutions were 0.3; 0.5; and 0.7, respectively. The surfactants mixtures were investigated at pH 6.0-6.5 and at constant ionic strength of the solution. The concentration of TX-100 and HDS in the probes were determined by the spectrophotometric and two-phase titration methods, respectively.

Adsorption isotherms of the individual surfactants and their binary mixtures on graphitized carbon black were obtained. Adsorption from binary surfactants mixtures is small at TX-100 content of $n = 0.3$. At a surfactant content of $n = 0.5$, adsorption increases due to formation of mixed TX-100 - HDS aggregates. At a high TX-100 content ($n = 0.7$), an increase in total surfactants adsorption value is mainly due to adsorption of the nonionic surfactant. HDS adsorption increase to a small extent at all investigated components ratios. When TX-100 contents in the binary TX-100 - HDS system are equal to $n = 0.5$ and $n = 0.7$, the experimental total adsorption values are larger than calculated ones for ideal systems. The maximum deviation from the ideal system is found at equimolar surfactants content in the binary mixtures. This might be explained by the fact that both surfactants molecules/ions and their mixed aggregates are capable to adsorb on carbon black surface.

The composition of the mixed adsorption layer on carbon black surface was calculated using the Ruben-Rosen theory and this composition agrees with the experimental data. The surfactant amount adsorbed on carbon black is larger comparing with one at the air-liquid interface due to dispersion interactions of the surfactants molecules with the sorbent surface.

Nonlinear diffraction of volume structures based on metal nanoparticles

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Periodic structures with noble metal nanoparticles (NP) are of scientific interest both for fundamental science and for applied tasks. Due to quantum size effects and local surface plasmons they have high nonlinear susceptibility and ultra-fast non-linear response. Such structures can be used sensors [1], as materials with variable electrical properties [2], optical constraints [3].

We used two types of photopolymerizable compositions for manufacturing of polymer-NP structures. In the first case, the *ex situ* synthesized Au NP were introduced into a monomer mixture. In the second case, the Ag NP synthesis occurs after the recording. Volume structure is formed as a result of local polymerization and diffusive redistribution of the mixture components in interference field. Nonlinear diffraction was investigated by measurements of the transmissing and diffracted beams and the method of recording dynamic gratings.

It is shown that nanocomposites containing Ag NP and diffraction gratings made on their basis are characterized by a negative sign of nonlinearity. For structures containing Au NP a cubic nonlinearity typical for Au NP is observed ($\chi^{(3)}$~ 11^{-8}). It is established that the nonlinear behaviour of diffraction efficiency from the intensity of the beam diffracted on the gratings is the result of the NP specific properties and depends on the NP size and concentration.

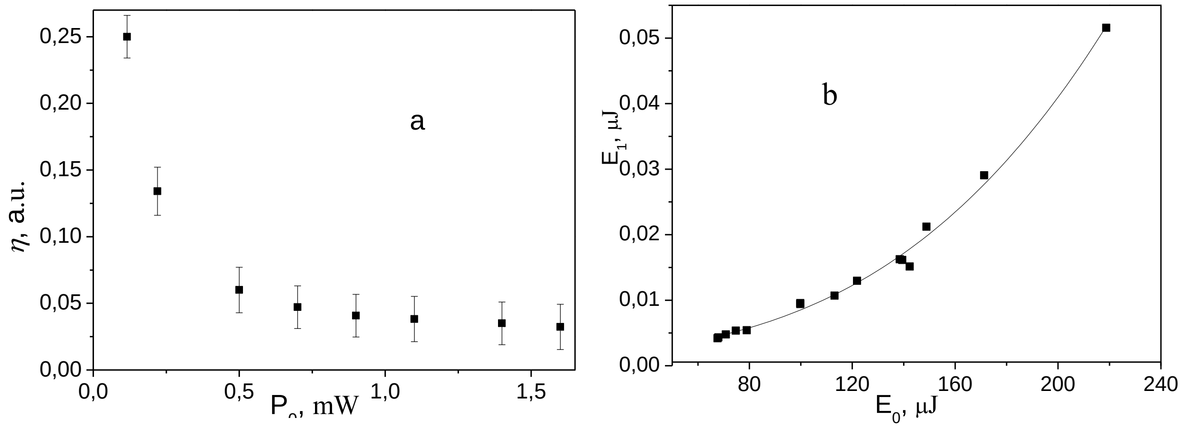

Fig. Nonlinear diffraction: *a*- periodic structure with Ag NP , *b*- nanocomposite with Au NP

1. C. Hanisch, A. Kulkarni, V. Zaporojtchenko, F. Faupel, J Phys.: **100 (**2008) 052043.
2. V. Pardo-Yissar, R. Gabai, A. N. Shipway, T. Bourenko, I. Willner, Adv. Mater. **13** (2001) 1320.
3. Y. Dirix, C. Bastiaansen, W. Caseri, P. Smith, Adv. Mater. **11 (**1999) 223.

Polyvinylidene fluoride membranes modification with TiO_2 nanoparticles

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Polyvinylidene fluoride membranes are widely used for water purification due to their properties, such as high mechanical strength, good thermal stability, and excellent chemical resistance. The main disadvantages of PVDF membranes is their low reactivity and high hydrophobicity, which leads to membrane fouling during filtration of proteins and polysaccharides solutions.

PVDF membranes were modified with TiO_2 nanoparticles to improve their properties. For this purpose, membranes were treated with polyethyleneimine in carbonate buffer at 55 ºC overnight. After that TiO_2 nanoparticles, stabilized by citric acid, were grafted to amino groups via peptide bond formation. Modification was confirmed by IR spectroscopy and electrokinetic analysis (Fig.).

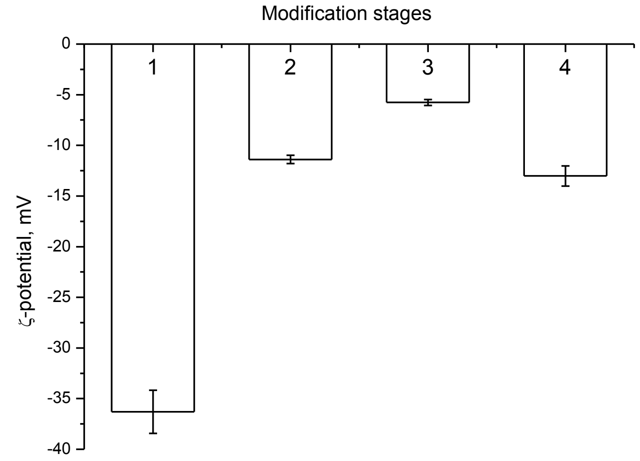

Fig. Changing of zeta-potential of PVDF membrane surface during modification: *1* – unmodified PVDF membrane; *2* – PVDF membrane treated with carbonate buffer; *3* – PVDF membrane treated with carbonate buffer with polyethyleneimine; *4* – PVDF membrane treated by carbonate buffer with polyethyleneimine with further grafting of TiO_2 nanoparticles

Zeta-potential of unmodified membrane was strong negative (-36.3 mV). After modification with polyethyleneimine it changed to slightly negative because of positive charge of amino groups (-5.8 mV). After grafting nanoparticles covered with citric acid zeta-potential was -13.0 mV.

So, proposed method of membrane modification allowed introducing functional groups and hydrophilizing the surface of PVDF membranes.

Symmetry properties of Brownian motors with fluctuating periodic potential energy

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Brownian particles, that diffuse in a spatially periodic potential under the action of an unbiased driving force, are a prototype of Brownian motors, model systems in which temporal fluctuations of the potential energy can initiate directed motion. The directed motion of a Brownian particle (motor) is possible if a number of the system's symmetry conditions are satisfied. Therefore, it is a fundamental importance to find the types of symmetries that exclude the emergence of direction motion, since real motors can function only if they are broken.

At present, the main types of symmetries are known, which were systematized and analyzed in Refs. [1, 2]. D. Cubero and F. Renzoni recently discovered a new type of the hidden symmetry for inertialess motion in dissipative systems [3]. Using the explicit analytical expressions obtained earlier for the velocity of Brownian motors operating in the high-temperature and adiabatic modes, we propose an alternative, more visual and effective, method to identify and analyze the types of space-time symmetry.

We consider the inertialess motion of a Brownian particle in a potential field described by an arbitrary periodic function of coordinate and time. The first terms of an expansion of the average particle velocity over the small parameter, which is the ratio of the amplitude of potential energy changes to the thermal energy, have been represented, that is, the expression for the high-temperature Brownian motor average velocity. The analysis of those terms revealed the vector and shift symmetry as well as the hidden space-time symmetry of Cubero-Renzoni. These symmetry types have been used to analyze space-time dependences of potential energy which prevent the appearance of the ratchet effect. We also study the additional types of symmetry, which are inherent in adiabatically slow and fast Brownian motors, as well as the conditions for the potential energy at which the average motor velocity becomes zero.

1. P. Reimann, Phys. Rev. Lett. **86** (2001) 4992.
2. S. Denisov, S. Flach, P. Hänggi, Phys. Rep. **538** (2014) 77.
3. D.Cubero, F. Renzoni, Phys. Rev. Lett. **116** (2016) 010602.

Piecewise-linear approximation of the potential relief of a Brownian motors

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The ratchet effect, that is the rectification of chaotic thermal motion into a directed one by organization of the blocking mechanism of multidirectional flows under certain conditions, plays the key role of the theory of Brownian motors [1-3]. For generation of these flows, it is necessary to organize a spatial asymmetry in the system, which can be realized with a piecewise linear sawtooth, periodic, and asymmetric profile. There are many implementations of the ratchet-mechanisms using the sawtooth (or similar to them) potentials: various on-off ratchets and their modifications, devices for separation of particles, two-dimensional ratchet-constructions consisting of sawtooth patterns, artificial protein ratchets, quantum ratches, *etc*. In the theory of Brownian motors, a sawtooth potential occupies important place too. First, it is simple in describing (this potential is characterized by only two parameters). Secondly, it consists of two linear sections, which allows analytical representations obtaining of the motor main characteristics, as well as using the transfer matrix method. Thus, it allows to estimate and predict the motor effect in many cases.

In this message, it proposed a convenient method to find the parameters of the sawtooth potential, which is closest to the given real one. Approximation of an arbitrary antisymmetric periodic function by a sawtooth potential is considered, and a general system of equations for finding its parameters is formulated. The proposed method is illustrated by the example of the sum of two sinusoids. It is shown that the applying of the sawtooth-potential approximation in the theory of Brownian motors is well suited in the high-temperature motion regimes.

1. P. Reimann, Phys. Rep. **361** (2002) 57.
2. R.D. Astumian, J. Phys. Chem. **100 (49)** (1996) 19075.
3. R. D. Astumian, Science. **276** (1997) 917.

Nanoscale anodization products of silicon carbide

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Electrochemical dissolution of a crystalline 3C-SiC in HF-containing media along with mesoporous SiC gave another product – carbon fluorooxide (CFO) nanoparticles [1].

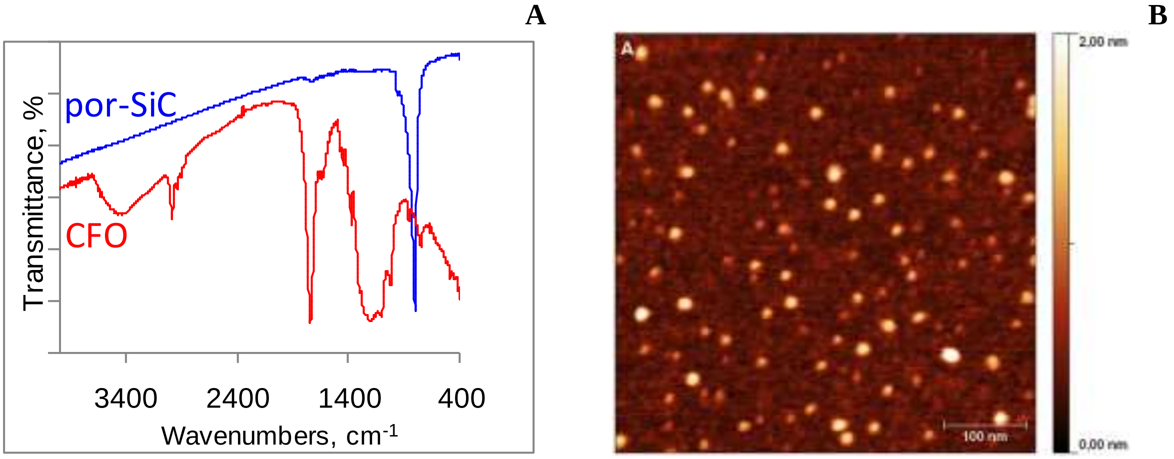

Fig. SiC etching products. *A* - FTIR spectra of a pure porous SiC and carbon fluorooxide nanoparticles (CFO); *B* - AFM image of CFO alone

Chemical nature of these products was studied by means of FTIR spectroscopy, temperature-programmed desorption mass spectrometry (TPD-MS), ^{1}H, ^{13}C, and ^{19}F NMR (liquid and MAS techniques), XPS, DLS, AFM and other methods.

CFO mostly consists of 1−10 nm nanoparticles/macromolecules and acts as a typical organic substance. A model of its chemical structure is a relatively small graphene domains interconnected with partially fluorinated hydrocarbon bridges and terminated by polycarboxylated alkyl chains (with carboxylic acid ($-CO_2H$) and ethyl ester ($-CO_2C_2H_5$) groups) and perfluorinated functional groups.

Presence of carboxylic acid functionalities endows CFO NPs with relatively high zeta-potential (*ca.* -40 mV) in aqueous media that stabilizes colloid solution and facilitates functionalization through amide chemistry (for instance, hydrophobization with long chain alkyls).

1. S. Alekseev, D. Korytko, M. Iazykov, S. Khainakov, V. Lysenko, J. Phys. Chem. C. **119** (2015) 20503.

Influence of structural organization of nanophase catalysts on their selectivity in deep, selective and preferential oxidation of CO and methane

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The perspective approach for achieving high selectivity of heterogeneous catalysts is multi-scale strategy successfully applied in modern nanomaterial studies. Solid material, in particular, a catalyst, is considered as a single system of interconnected components, characterized by macro-, micro, nano-and molecular structural levels. The determining influence on the functional properties (activity, selectivity, chemical and thermal stability) has the structural organization of active centers on the surface attributed to the nano and molecular levels.

According to this approach, the structural organization of nanophase catalysts for CO and methane oxidative conversions is investigated. The basic principles, binding the structural organization of nanophase catalysts and their selectivity towards deep CO and methane oxidation to CO_2, the methane oxidative carbonylation into acetic acid and preferential CO oxidation in hydrogen (PROX) are established. The contribution of electronic and geometric effects arised from changing size characteristics in nanometer range are taken into consideration.

It is shown that the main factor determining the selectivity is the structural organization of the active center located on catalyst surface, characterized by common features for each type of reaction, regardless of the chemical nature of the catalysts components.

A new approach to the development of selective oxide catalysts for the preferential oxidation of CO in hydrogen by integrating nanophase components into a spatially organized system is proposed [1]. It is found that the selectivity of the supported Cu-CeO_2/ZrO_2 catalysts in PROX process depends on the textural characteristics of zirconia. The most active and selective is catalyst supported on a high temperature zirconia, that caused by the formation a large number of active sites of CO oxidation performed by Cu-Ce contact zones.

1. G.R. Kosmambetova, Theor. Exp. Chem. **50** (2014) 265.

Metal oxide-carbon hybrid nanomaterials for stable electrocatalysis in solid acid fuel cells

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Fuel cells have the potential to be a key technology meeting the still increasing energy demand created by our modern world. Besides cost factors, the long-term stability is a central issue hindering their widespread commercialization [1]. This especially applies to nanostructured materials used in state of the art electrodes [2, 3].

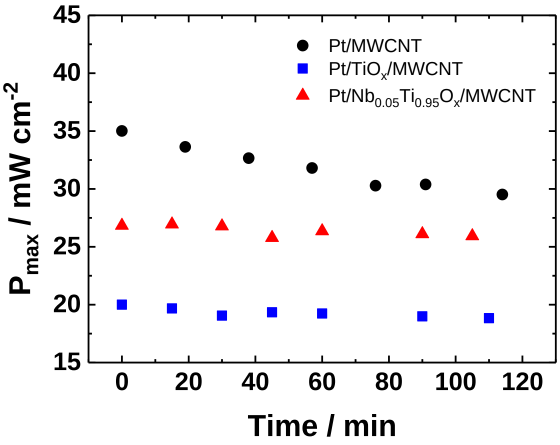

Fig. Peak power density as function of operation time of prepared solid acid fuel cells

In this work, nanostructured carbon-based substrates, serving as catalyst support and current collector, were coated with a thin metal oxide layer to improve their stability in solid acid fuel cell cathodes. The coating was synthesized by a photochemical approach and extensively characterized. Fuel cell measurements show a significant improvement regarding degradation resistance of the coated nanomaterial as compared to the uncoated one (Fig.).

1. P. Trogadas, T.F. Fuller, P. Strasser, Carbon **75** (2014) 5.
2. E. Antolini, Appl. Catal. B **88** (2009) 1.
3. Y.-J. Wang, B. Fang, H. Li, X.T. Bi, H. Wang, Prog. Mater. Sci. **82** (2016) 445.

Radio-absorbing materials with adjustable dielectric properties

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It is known that radio-absorbing materials (RAM) are structural dielectrics that effectively absorb the electromagnetic energy of radio waves. According to the classification, radio-absorbing materials can be magnetic and non-magnetic. In turn, non-magnetic radio-absorbing materials are subdivided into gradient, interference and combined. Gradient RAM have a multilayer structure (see Fig. 1) with a smooth change of the value of dielectric permeability along the thickness of the material $\varepsilon_1 > \varepsilon_2 > \varepsilon_3 > \varepsilon_n$. The first layer of RAM should be made of a material having low dielectric losses (ε_1) in order to match the wave resistance of air and material (for example, celsian and slavsonite). Other layers are made of solid dielectrics with high dielectric permeability (ferroelectrics, ferroelectromagnets and others), and also with the use of magnetic or non-magnetic radio-absorbing fillers, which are introduced into the dielectric matrix (graphite, ferrites and others).

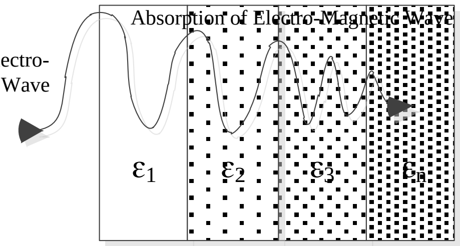

Fig. 1. Schematic view of the gradient radio-absorbing material

The work done allowed to solve the problem of obtaining a ceramic material based on the $SrO–TiO_2–SiO_2$ system (see Fig. 2) with high values of the permeability.

On the basis of the studies carried out, a technology for manufacturing a ceramic material of composition II (SiO_2 – 1.97, TiO_2 – 45.40, SrO – 52.63) with a high dielectric permeability was developed. The technology of manufacturing ceramics based on strontium titanate consisted of two stages. The first stage of synthesis occurred at a maximum temperature of 1300 °C with holding during 2 hours. The second stage was carried out at a temperature of 1330 °C with holding for 1 hour. It was found that the composition II has the best indicators (firing temperature 1330 °C), which is located in the triangle Sr_3T_2 – SrT – SrS with the following properties: dielectric permeability $\varepsilon = 115$; water absorption *W*,% – 1.3; open porosity *P*,% –5.8; density ρ, g/cm^3 – 4.35.

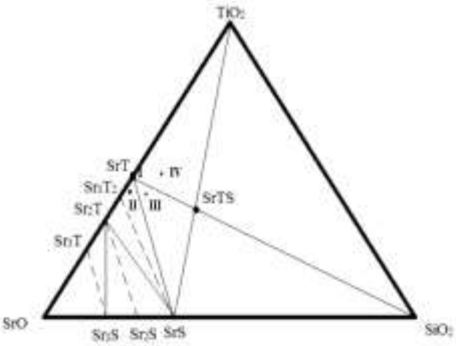

Fig. 2. Diagram of the three-component system $SrO–TiO_2–SiO_2$

The generalization of the obtained data allows to draw a conclusion that the developed composition of the ceramic material on the basis of the three-component system $SrO–TiO_2–SiO_2$ is promising for creating a gradient radio-absorbing material.

Thermal transformation of cinnamic and aliphatic carboxylic acids on the nanoceria surface

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Catalysis and catalytic pyrolysis have been widely used in biomass conversion technology and upgrading of bio-oil [1-2]. Catalytic conversion can be utilized to biomass to produce high value added chemicals. Cinnamic and fatty acids in the form of lignin and triglycerides are the parts of the biomass. Lignin polymers are composed of heterogeneous aromatic monomeric units of cinnamic acids (coniferyl-, sinapyl-, and *p*-coumaryl-units) cross-linked via a variety of chemically stable bonds. Therefore, the thermochemical studies of small biomass units are important for development of biomass conversion technologies. In this work, thermal transformations of cinnamic and fatty acids on the nanoceria surface were compared by using temperature programmed desorption mass spectrometry (TPD MS) and FTIR spectroscopy.

The TPD MS experiments were performed on a MKH-7304A monopole mass spectrometer (Sumy, Ukraine) with electron impact ionization adapted for thermodesorption measurements. The non-isothermal kinetic parameters of the reaction of thermal decomposition (T_{max}, n, $E^{\neq}$, ν_0, and $dS^{\neq}$) were calculated from TPD MS data [3].

The main pathway of fatty acids transformation on the nanoceria surface is ketonization with the formation of symmetric ketones and carbon dioxide. Cinnamic acids surface complexes attached through carboxylic group decompose due to decarboxylation with the release of carbon dioxide and corresponding substituted vinyl benzenes (for example 2-methoxy-4-vinyl-phenol, 2-hydroxy-4-vinyl-phenol, vinyl-benzene, *etc*.).

Acknowledgements
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1. G.T. Neumann, J.C. Hicks, ACS Catalysis. **2** (2012) 642.
2. D. Mohan, C.U. Pittman, P.H. Steele, Energy Fuels **20** (2006) 848.
3. K. Kulyk, B. Palianytsia, J.D. Alexander, L. Azizova, M. Borysenko, M. Kartel, M. Larsson, T. Kulik, ChemPhysChem. **18** (2017) 1943.

Study of the thermal stability of nitrogen-containing graphene by using TPD-MS

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Thermochemical studies of CNT and graphene-based materials are important for their application in the electrocatalysis. Studies of the degradation of carbon nanomaterials are extremely rare, and their suitability for reliable electrochemical applications is largely not studied in the literature [1]. In this work, thermal stability of N-doped graphene were studied by temperature programmed desorption mass spectrometry (TPD MS).

The TPD MS experiments were performed on a MKH-7304A monopole mass spectrometer (Sumy, Ukraine) with electron impact ionization adapted for thermodesorption measurements [2]. The non-isothermal kinetic parameters of the functional groups decomposition, such as the temperature of the maximum desorption rate T_{max}, the reaction order n, the activation energy $E^{\neq}$, the pre-exponential factor ν_0 and activation entropy $dS^{\neq}$, were calculated from TPD MS data [2].

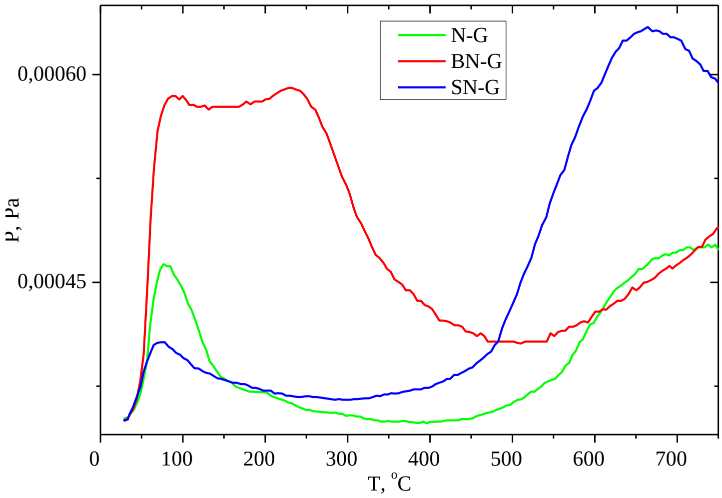

Fig. Vapor pressure measured as a function of temperature (P-T) for the samples of the N-doped graphene

Acknowledgements
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1. O. Naumov, F.P. Lohmann, B. Abel, A. Varga, ChemElectroChem. **4** (2017) 1306.
2. T.V. Kulik, J. Phys. Chem. C. **116** (2012) 570.

Hierarchical zeolites with BEA, MFI, MTW and MOR topology overgrown on expanded obsidian or perlite

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Hierarchical zeolites are materials in which orderly combined two or more types of pore systems, for example zeolitic micropores and transport mesopores. The latter facilitate the transport of molecules to active centers and reduce diffusion limitations, what allow to expect high activity of such materials in different acid-base and redox process including “bulk” (with diameter more than 1 nm) molecules. At the same time, these materials are quite expensive for use in industry. Synthesis of hierarchical zeolites overgrown on obsidian or perlite could significantly reduce the value of such materials.

Structured hierarchical zeolites overgrown on expanded obsidian or perlite were obtained using Gemini-type surfactants as structure directing agents (SDA) and this aluminosilicates as unique Al source. Si/Al ratio change was achieved by preliminary acid treatment of starting perlite and obsidian.

Structured hierarchical zeolites with MTW, MFI, MOR or BEA topology (as pure phases) were obtained varying of hydrothermal treatment time, SDA structure, and Si/Al ratio. Obtained materials consist of amorphous aluminosilicate (perlite or obsidian) phase on the surface of which zeolite nanosheets of 2 – 10 nm thickness are overgrown. Values of external surface were quite high and achieved 200 $m^2 \cdot g^{-1}$, while mesopore volume varied in range 0.25 − 0.6 $cm^3 \cdot g^{-1}$. It was established that degree of perlite or obsidian transformation into zeolite was increased with prolongation of time hydrothermal treatment and decrease of Al content in dealuminated obsidian and perlite.

All synthesized zeolites contain in structure Brønsted (BAS) and Lewis acid sites (LAS), which concentration varied in range 40 – 200 $\mu mol \cdot g^{-1}$. Concentration of BAS and LAS significantly depended on amount of amorphous phase in obtained structured hierarchical zeolites. Such materials will be tested as catalyst for different acid-base process.

Luminescent materials based on organic salts pyrolyzed at the silica surface

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Recently, carbon-based nanomaterials (nanodots) became highly attractive due to their low toxicity, good biocompatibility, chemical inertness, high photostability and fluorescence. These materials are thus potential candidates for using them as efficient nonoprobes, biovisualizers and phosphors. Doping with some heteroatoms, namely nitrogen, sulfur and silicon, was found to be an effective approach to improve their luminescence. One of the cheapest ways to obtain such nanomaterials is pyrolysis of N- and/or S-containing organic compounds, in particular organic salts. Besides, using the surface of inert material (for instance, silica) as a support can facilitate the nanodots formation by preventing the agglomeration during pyrolysis. The aim of this work was to study the luminescent properties of the materials obtained by pyrolysis of organic salt, namely citric acid ureate, at the silica surface depending on the citric acid:urea ratio and the solvent used for salt formation.

Fumed silica with a specific surface of 300 m^2/g was used as a support material. The salts with various ratios of citric acid and urea were obtained either in aqueous or alcohol solution, and they were further applied to silica surface by dropwise addition of the salt solution to a silica powder at high agitation speed in a reactor. The obtained powder-like material was dried and then thermally treated at the temperature of up to 270ºC. After that, the absorption and photoluminescence spectra for dried and pyrolyzed samples were collected and analyzed.

The results have shown that irrespective to the solvent used, both dried and pyrolyzed samples possess the luminescent properties. The change of the citric acid-to-urea ratio in aqueous solution within 1:(1÷3) doesn’t affect the luminescent properties of dried samples, but further pyrolysis at 270ºC reduces the photoluminescence intensity. The solvent change to alcohol has an ambiguous influence on the luminescent properties of dried silica samples with different citric acid-to-urea ratio applied, however, further thermal treatment at 270ºC results in the formation of the materials with almost the same luminescence properties. Within the citric acid-to-urea ratios and the solvents used, as well as the thermal treatment regimes applied, the variant with the 1:1 salt in the alcohol solution applied to the silica surface with further drying and thermal treatment at 270ºC was found to be the most suitable.

The relationship between the physical and chemical properties of polymer nanodisperse systems

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Considering the structural organization of flexible-chain polymers and heterogeneous composites on their basis as a set of certain subsystems, it was established that between viscoelastic (G-shear modulus, K-volume module, E-Young's module) properties, boundary of material strength (σ_M) and an effective coefficient of thermal conductivity (λ) there is an analytic dependence of the type $\sigma_i \sim \lambda^{1/2}$ (where $i = E, \sigma, K, \sigma_M$). The established dependence is obtained based on the model that a complex of properties of a composite can be described with the help of relaxation times, which depend on the frequency, temperature, type and content of the ingredients. The dependence of the thermal conductivity on the value of the bond energy on the boundary between the metal-polymer separation, the quasi-equilibrium distance between the structure formation of the material, is investigated. This model allows us to explain the relationship between λ and the temperature coefficient of the volume expansion of the system at $T \leq T_g$ (where T_g - the temperature of the glass material). In this connection, the relationship between the thermal and mechanical properties of PVC systems is also obtained on the basis of the free energy $F(T)$ by Helmholtz, depending on the type and content of the nanodispersed filler. It was established that an increase in the mechanical strength and thermal conductivity of composites occurs when the effective distance between nanoparticulate metal filler particles in the series: Cu, Fe, NiCr is reduced for ϕ, φ = const. On the condition that the polymer nanocomposite possesses a variable acoustic resistance due to the processes of scattering, refraction, dissipation and dispersion of acoustic waves, in the megahertz frequency range, on the basis of statistical analysis, experimental data it is established that between σ_M, the ultrasound velocity υ with longitudinal. There are quantitative interconnections between the capacitance and the deformation of the displacement and the coefficient of their absorption. Using the correlation analysis method, it is shown that $\sigma_M = A\upsilon^n\alpha^{-m}$. So, for PVC + 0.8 vol. % NiCr ($\phi = (35 \pm 2)$ nm) $n=2$; $m=3$. For any other nanocomposites obtained on the basis of flexible chain polymers, the coefficients for the indicated dependence can also be obtained using the Gauss method. It is shown that one of the correlation parameters is also the density of the composite. Possibilities of forecasting of the complex of properties of polymer systems and the area of their use are established.

Adsorption of natural cinnamic acids on the nanoceria surface

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Nanoceria (cerium oxide nanoparticles) shows unique biochemical properties and its efficacy in neutralizing biologically generated free radicals is perspective for biological and clinical applications. For the targeted delivery of cerium dioxide to damaged cells and organs certain biologically active substances must be immobilized on the surface of its nanoparticles. Natural plant antioxidants – cinnamic, coumaric, ferulic and caffeic acids are promising for this purpose due to the wide range of their pharmacological properties.

The purpose of the work was to determine the patterns of adsorption interactions between nanoceria and structurally similar cinnamic acids in dependence on their chemical structure at the physiological pH values of aqueous solutions. The type-S isotherm was found for the adsorption of cinnamic, 4-hydroxycinnamic (coumaric) and 3-methoxy-4-hydroxycinnamic (ferulic) acids on the nanoceria surface, whereas the 3,4-dihydroxycinnamic (caffeic) acid adsorption is described with the type-H isotherm which is typical for the chemisorption. Strong correlation between adsorption values corresponding to the initial parts of S-isotherms and the hydrophobicity parameters (log *P*) testifies plane position of adsorbed molecules on the sorbent surface. The maximum values of acids adsorption ($\sim 2.9 \cdot 10^{-4}$ mol/g) correlate with the values of their thermodynamic dissociation constants ($pK_{COOH} = 4.4 - 4.6$) that is possible on condition of acid molecules vertical orientation on the surface.

The pH-dependence of cinnamic acids adsorption has bell-shaped form which maximum correlates with pK_{COOH} values. The presence of a hydroxyl group in the molecules of coumaric, ferulic and caffeic acids leads to the extension of the pH-interval of their adsorption in comparison with cinnamic acid.

Adsorption interaction of hydroxycinnamic acids with nanoceria is accompanied by appearance of new absorption bands at > 360 nm characteristic for each acid. The intensity of sorbent colour is proportional to the surface concentration of coumaric, ferulic and caffeic acids and can be assessed visually. This is promising for the development of simple visual test systems for evaluation of hydroxycinnamic acid antioxidant activity, particularly, in the field.

Electrophysical properties of carbon nanotubes / NiCo composites

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To date, a lot of composite materials (CM) on the basis of carbon nanotubes have been synthesized for obtaining electromagnetic devices, catalysis, antifriction, anticorrosion coatings, and others.

The purpose of this work is to synthesize composites of multilayer nanotubes/NiCo (MWNT/NiCo) and to establish differences in their electrophysical properties, depending on the nature of the surface.

Two consignments of MWNT/NiCo composites were synthesized using conventional and oxidized MWNT. Synthesis was carried out by the method of co-precipitation from a solution of hydrazine hydrate of nickel, cobalt and aqueous suspension of nanotubes. The suspension was pre-treated with ultrasonic dispersant.

The CM were investigated using an electron microscope, X-ray diffraction and electrophysical methods in the high and low frequencies. Investigation of the real (ε') and the imaginary (ε'') components of the complex dielectric permittivity of composites was made in ultra-high frequency (UHF) ranging 8-12 GHz and using an interferometer РФК-18 which was based on measuring the phase difference. Standing wave ratio and the weakening of R2-60 by the no-electrode method. And the conductivity was made at low frequencies of 0.1. 1 and 10 kHz were made with two-contact method using immittance meter E7-14. The results are presented in the Table.

Table. Electrophysical characteristics of MWNT/NiCo composites

	Complex permittivity in the range of 8-12 GHz		Magnetic permittivity on frequency 8 GHz		Conductivity σ on 1 kHz, $Ohm^{-1}cm^{-1}$
	ε′	ε″	μ'	μ″	
Non oxidized MWNT/NiCo	7.3	6.9	2.9	2.2	2.9
Oxidized MWNT/NiCo	7.5	6.4	3.1	2.5	1.6

The corresponding values of electrophysical characteristics differ slightly, but beyond the limits of the error due to similar composition and technology for obtaining nanocomposites. The difference in characteristics can be attributed to the additional treatment of MWNT and the presence of a significant number of functional bonds on the surface. MWNT, due to oxidation, have less electrical conductivity, but the better magnetic properties are on microwave.

Optical studies of CdSe nanocrystals grown from aqueous solutions in the presence of gelatine

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Due to pronounced size quantization, CdSe nanocrystals have become an object of extensive research in view of fundamental physical effects observed as well as targeted applications as active media for optical and optoelectronic devices, solar cells, fluorescent labels in biophysical experiments *etc*. Size-dependent characteristics of CdSe nanocrystals, especially photoluminescence (PL) spectral position, intensity and halfwidth, can be effectively varied across a broad spectral range. Here we report on CdSe nanoparticles synthesized at relatively mild conditions from aqueous solutions in the presence of gelatine and characterized by optical absorption and PL spectroscopy.

CdSe NCs were obtained in aqueous solutions by decomposing a cadmium(II) complex with selenosulfate anions in the presence of 5% gelatine (or gelatine+polyvinylpirrolidone mixture) and subsequently deposited on glass substrates. The resulting 0.15–0.22 mm thick films contained CdSe NCs evenly dispersed in organic polymer matrices.

Optical absorption spectra of the films obtained were measured using a Cary 50 spectrophotometer (Varian) with a full spectrum Xe pulse lamp single source and dual Si diode detectors. PL measurements were performed using a DFS-24 double monochromator with excitation by a solid-state laser (405 nm).

The absorption spectra enabled us to judge upon the average size of the CdSe nanocrystals and its dependence on the preparation conditions, especially on additional heating of the reaction mixture. The dependence of the PL intensity, width and spectral position on the preparation conditions is analysed. Optimization of conditions resulting in the preparation of the samples with the narrowest size distribution as well as good tunability and high intensity of the PL is discussed.

Long-term stability of sodium oxygen batteries

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Sodium oxygen (Na-O_2) batteries are a potential candidate for the application in electrical vehicles [1]. They combine high theoretical energy density with relatively cheap materials and feasible round-trip efficiency. However, the limited cycling life hinders their commercialization.

In this work, the electrochemical cell performance of a self-assembled Na-O_2 batteries are investigated. During the discharge the battery ages which leads to a continuously drop of the discharge potential. Therefore, the electrochemical stability in nitrogen or oxygen gas flux has been tested with electrochemical impedance spectroscopy. A potential reason for the aging might be the passivation reaction at the anode. Oxygen could diffuse through the electrolyte and react with the sodium anode resulting in an increased internal cell resistance.

Additionally, the discharge product contribution at the cathode has been analyzed with the photometric reaction of Ti(IV)-ions with the discharged products. Approximately 30% of the electrochemically deposited discharge products were detected photometrically. The discharge products have their maximum at the outermost annulus and decrease discontinuously till the minimum at the innermost annulus. The reasons are the asymmetric cell geometry and the geometry of the spring.

Moreover, the conductivity of sodium *bis*(trifluoromethansulfon)imide (NaTFSI) was compared with sodium trifluoromethansulfonate (NaOTf) and sodium hexafluorophosphate ($NaPF_6$) in an diglyme or an tetraglyme electrolyte, respectively. NaTFSI has the highest conductivity compared to the same concentration of $NaPF_6$ and NaOTf in diglyme and tetraglyme, correspondingly.

1. H. Yadegari, Q. Sun, X. Sun, Adv. Mater. **28** (2016**)** 7065.

Removal of trace amount of dyes from aqueous solution by polyfunctional N-, P-, S-containing silica

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The world industry (metallurgical, leather tanning, textile *etc*.) produces many types of waste streams. The determination of toxic pollutants in real samples is challenging because of their low concentration and the complexity of wastewater matrix. The most important technologies for the removal and separation of toxic compounds including organic dyes in aqueous solution are biological degradation and oxidation, chemical precipitation, membrane filtration and adsorption. Nevertheless, adsorption is an old, simple yet effective method, among the wide range of selective technologies applied to remove both dyes and heavy metals efficiently without special facilities [1].

The main objective of this study was applied polyfunctional -NH-P(S)(OC_2H_5)$_2$/-SH silica for the selective removal of the trace amount of organic dyes from water samples followed by UV-Vis spectroscopy. Here, Methylene Blue is selected as the model target pollutant science it chemical behaviour is similar to other organic dyes (Fig.).

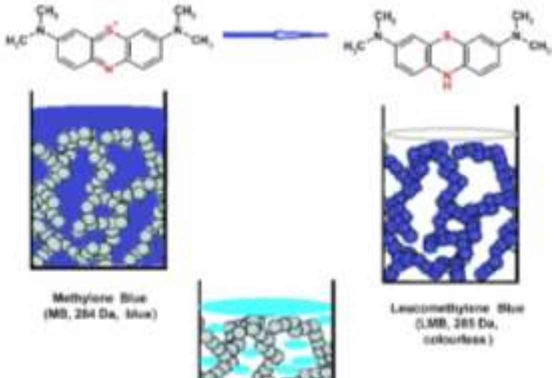

Fig. Discoloration of the dye under the action of functional groups of the surface of –NH-P(S)(OC_2H_5)$_2$/-SH silica

1. J. Fan, J. Mater. Chem. A. **4** (2016) 3850.

Interaction of β-cyclodextrin with 2,4-dihydroxybenzoic acid in aqueous solutions

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Cyclodextrins (CD) are used for chromatographic separation and purification of organic compounds, extraction and concentration of impurities of toxic substances, decreasing the toxicity of drugs, as well as in the synthesis of selective sorbents and sensors.

2,4-Dihydroxybenzoic acid (DHBA) refers to phenolic compounds which even at low concentrations harmfully affect living organisms.

DHBA is used in the synthesis of pesticides, herbicides, organic resins, plasticizing additives, colorants. The main sources of DHBA entering the water basin are industrial wastewater, agricultural land drains and effluents of inefficient treatment facilities. Therefore, the development of new effective methods of water purification to remove DHBA, as well as quantitative analysis methods to determine its content in aqueous solutions, are of great importance.

The interaction of β-CD with DHBA was investigated in aqueous solutions with pH 1.0 and 4.0. The composition of complexes and their stability constants were determined using the Benesi–Hildebrand method. The formation of 1:1 “host – guest” inclusion complexes between β-CD and the molecular form of DHBA (or its monovalent anion) was proved. It was fixed that the inclusion complex of uncharged form of DHBA with β-CD exhibits higher strength.

The change in the Gibbs free energy for the process of formation of the complex of β-CD with DHBA was calculated by the equation $\Delta G^{o} = -RT \ln Ks$, the enthalpy and entropy values were determined graphically using equation $\ln Ks = \Delta S^{o}/R - \Delta H^{o}/RT$.

The nature of the change in the thermodynamic parameters of complex formation indicates a spontaneous exothermic process of formation of new supramolecular structures in the β-CD – DHBA system. It was proved that inclusion complexes are formed due to van der Waals interactions between the aromatic ring of DHBA and the internal hydrophobic cavity of β-CD. The obtained results can be used to predict the efficiency of extraction of DHBA from water and aqueous solutions using cyclic oligosaccharides and functional β-cyclodextrin-containing materials.

Organometallic composites with catalytic properties based on TEOS and transition metal salts

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Nanoparticles of metal oxides coated by silicon oxide with paramagnetic properties can serve as the basis for the synthesis of various catalytic systems. In work, pre-obtained composites $CoFe_2O_4/SiO_2$ with a developed surface were used as the basis, on which $CuO/SiO_2/CoFe_2O_4$ catalytic systems were synthesized.

Nanosized catalysts based on copper oxide were obtained by the method of precipitation from a solution of copper hydroxide with sodium hydroxide solution. As the centers for $Cu(OH)_2$ precipitation $CoFe_2O_4/SiO_2$ composites were used. They were synthesized by two-stage technique: at the first stage, the precipitation of cobalt and iron hydroxides from the solutions of their salts took place, which in the second stage served as SiO_2 precipitation centers at the sol-gel transition of TEOS. In the first case (sample No.1), particles pre-calcined at 400°C to the formation of complex oxide $CoFe_2O_4$ were used. In the second case (sample No.2), $CoFe_2O_4/SiO_2$ composites were used as the centers of $Cu(OH)_2$ precipitation after rinsing without calcination. The verification of the catalytic action of the obtained systems on the process of cumene oxidation by molecular oxygen was carried out. For comparison, processes of cumene without catalyst and using as a catalyst $Cu(NO_3)_2/SiO_2$ composite, obtained by adsorption of a copper salt by SiO_2 nanoparticles, previously synthesized by sol-gel method during alkaline hydrolysis, were caried out (sample ADS $Cu(NO_3)_2$).

Table. The rate of initiated cumene oxidation

No	AIBN, mol/L	ADS $Cu(NO_3)_2$, g/g	No.1, g/g	No.2, g/g	$W\cdot10^5$, mol/L·s
1	0.02	–	–	–	1.9
2	0.02	0.005	–	–	6.5
3	0.02	–	0.005	–	9.01
4	0.02	–	–	0.005	15.7

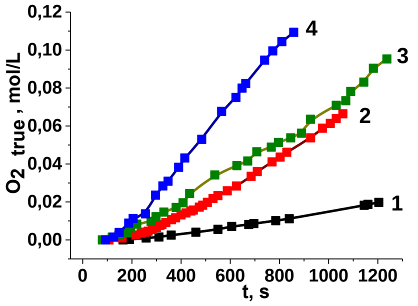

Fig. Kinetic curves of the process of cumene oxidation by molecular oxygen without a catalyst and with different catalysts

The use of $CuO/SiO_2/CoFe_2O_4$ composites as catalysts makes it possible to increase the reaction rate by 6-8 times, which indicates their prospects for this process. These investigations showed the possible use of organometallic composites of sol-gel systems on the basis of TEOS and transition metal salts as catalysts in the reaction of cumene oxidation with molecular oxygen.

Physical-chemical technologies for the production of metal-dispersed polymer systems

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New methods for the creation of high-performance ferro- and para-diamagnetic materials, which serve as nanodispersed fillers of flexible-chain polymers, are developed and presented. In particular, methods have been proposed: an electrical explosion of a conductor (EEC); physical-chemical (ph/ch) dispersion; electrodeposition of ferromagnetic nanodispersed metal powders by an electro-ultrasonic field (e/u) in the cavitation mode, chemical (e/ch) reduction of ferromagnetic metal salts from aqueous solutions. The developed methods give an opportunity to get in the reactor the combination of a polymer matrix with a nanodispersed metal, and then in the T-p mode composite. In this case, a new mechanism for transferring ions and the action of specific acoustic effects (sound wind, radiation pressure, cavitation) have been established, which increase the kinetic energy of charged nanoparticles of a metal.

The influence of the volt-ampere regime of the EEC on the final output of the metal, acoustic factors on the process of fragmentation of microparticles and the electrodeposition of nanodispersed metal is investigated. It is established that the intensity of the ultrasonic field and its frequency influence strongly on the structure of nanodispersed metal and composite.

Particular attention is paid to nanodispersed particles of iron and carbon. It is shown that the complex (physical-mechanical and thermophysical) properties of a composite with a modifier content in the range of $\varphi \geq (0{,}06 \div 0{,}08)$ vol.%, substantially changes at approximation of their size to the critical one. The viscoelastic, electrophysical and magnetic properties of composites obtained on the basis of PVC, PS, containing nanodispersed Fe, NiCr and carbon nanostructured fillers have been investigated. It is shown that the process of percolation, as well as the magnetization of the system, depends on the size of the nanoparticles, having a tendency to intensively reduce the effect. By extrapolation, depending on the physical and chemistry of the surface, the critical (minimum) dimensions of the ingredients are defined as a necessary condition for intensifying the properties of the material.

Tungsten carbide based cathodes modified with titanium or hafnium for hydrogen evolution from water

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Tungsten monocarbide (WC) features a high electrocatalytic activity in hydrogen discharge-ionization in acid solutions. Cathodes, based on WC fine powder, can be recommended for hydrogen evolution from acid solutions instead of ones, containing platinum catalysts. In the present work, WC-based cathodes were modified with titanium or hafnium for further increasing their electrocatalytic activity.

The cathodes were prepared by fritting a mixture of fine metal powders (WC + 10 wt. % Ti or Hf) with water solution of polyvinyl alcohol on a nickel mesh at 1100 ºC under argon. Polarization curves (2 mV/s) of hydrogen evolution at the prepared cathodes were taken in 1 M H_2SO_4 at 25-70 ºC.

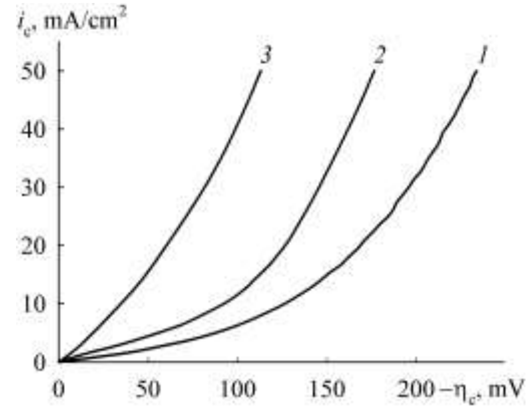

Fig. 1. Polarization curves of hydrogen evolution from 1 M H_2SO_4 (55 ºC) at the following cathodes: *1* – WC; *2* – WC + Ti; *3* – WC + Hf

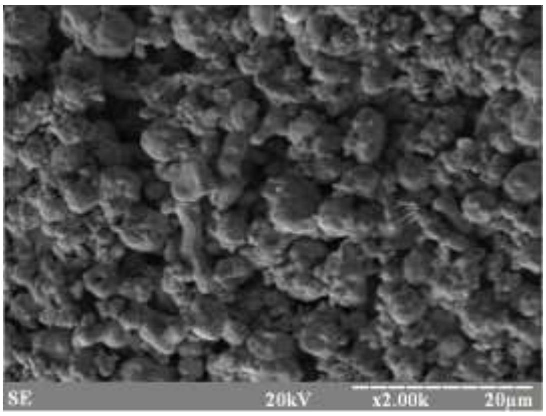

Fig. 2. Surface micrograph (× 2000) of WC + Hf cathode after polarization measurements

It has been found that doping a WC powder with a Ti or Hf powder resulted in significant decrease in hydrogen evolution overpotential, especially when WC was doped with Hf (see Fig. 1). Exchange current density of the WC + Ti and WC + Hf cathodes at 55 ºC amounted to $9.9 \cdot 10^{-4}$ and $4.7 \cdot 10^{-3}$ A/cm^2, respectively. Therefore, WC + Hf cathodes were most active in the hydrogen evolution reaction among other investigated cathodes.

The surface of prepared fritted WC-based cathodes was developed and nonuniform even after polarization measurements (see Fig. 2).

Pyrimidine nucleotide complexes on the nanocrystalline titania surface

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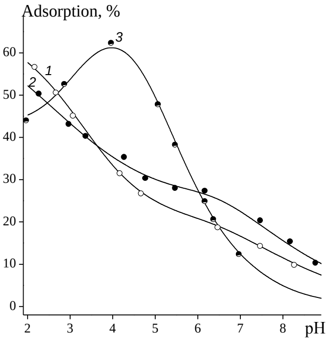
The interface between biomolecules and inorganic oxide surfaces has attracted considerable attention as a decisive factor in bioapplication of nanosized oxides. To define interaction of oxide nanoparticles with a biological medium is an extremely complex task. One of the approaches to solve this problem is the way of model studies of the interaction of individual biomolecules with oxide surfaces. The adsorption of monophosphates of cytidine (CMP), uridine (UMP) and orothidine (OMP) from aqueous solutions on the surface of nanocrystalline titania was studied. The interaction of pyrimidine nucleotides (PNP) with hydroxyl groups of titania is interpreted in terms of the surface complexation theory. Experimental data obtained in the study of the adsorption as function of pH and ionic strength were used to calculate the stability constants of outer-sphere adsorption complexes that are formed due to electrostatic interaction of protonated $TiOH_2^+$ groups with anionic nucleotide forms. To quantify the protolytic properties of TiO_2 and adsorption equilibria involving organic molecules, the basic Stern model for double electric layer and GRFIT program were used.



Adsorption of OMP (*1*), UMP (*2*), and CMP (*3*) from 0.01 M NaCl solution:
C_{PNP}=0.1 mM, C_{TiO2}=1 g/l

Thus, for cytidine-5'-monophosphate, the best fit of the experimental data and the calculated adsorption curves was obtained under the assumption of several complex formation reactions:

$$\equiv TiOH + H_2L^{\pm} + H^+ \leftrightarrow \equiv TiOH_2^+ H_2L^{\pm}, \quad \lg K_{1S} = 9.98 \pm 0.06;$$

$$\equiv TiOH + H_2L^{\pm} \leftrightarrow \equiv TiOH_2^+ HL^-, \quad \lg K_{2S} = 5.53 \pm 0.05;$$

$$\equiv TiOH + H_2L^{\pm} \leftrightarrow \equiv TiOH_2^+ L^{2-} + H^+, \quad \lg K_{3S} = -0.52 \pm 0.05.$$

To test the assumption that the most probable nucleotide binding center with protonated groups on the TiO_2 surface is phosphate anion, the adsorption of inorganic phosphate from aqueous solutions was studied.

Our experimental data are interpreted as the result of the formation of electrostatic outer-sphere complexes $\equiv TiOH_2^+ H_2PO_4^-$ ($\lg K_{1S} = 9.68$) and $\equiv TiOH_2^+ HPO_4^{2-}$ ($\lg K_{2S} = 4.69$).

Thus, the comparison of adsorption curves for pyrimidine nucleotides and inorganic phosphate leads to the conclusion about the electrostatic nature of the interaction between active surface centers and phosphate anions.

Electrophysical characteristics of polymer nanocomposites based on carbon nanotubes/ferrites modified copper iodide

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Relevance is caused to the special functional properties of materials, such as oxide ferromagnets and solid solutions based on them. These materials are used in various fields, as magnetic field sensors, magnetic memory devices, microwave devices, magnetophotonics, *etc*.

In order to create the new nanomaterials that effectively interact with electromagnetic radiation, nanocomposites such as carbon nanotubes (CNT)/barium ferrite precursors (BFP) were synthesized by the sol-gel autocombustion method, and the volumetric CNT content was ≤ 0.11. $Ba(NO_3)_2$ and $Fe(NO_3)_3 \cdot 9H_2O$ were dissolved in distilled water. The Ba^{+2}/Fe^{+2} molar ratio was adjusted at 1:12. The citric acid was used as a chelating agent. The suitable amount of ammonia was added drop-wise in the solution to adjust the pH approximately 7. CNT were pre-dispersed by ultrasound in distilled water and added in the above solution. Barium ferrite precursors were heat-treated at 673 K for 8 h (CNT/BFP–*h*). The samples CuI/CNT/BFP and CuI/CNT/BFP–*h* were prepared by a chemical method during the course of release of CuI from an aqueous solution of $CuSO_4$ and KI, $Na_2S_2O_3$ in the presence of CNT/BFP. The samples of system CuI/CNT/BFP–polychlorotrifluoroethylene (PCTFE) were compacted at the temperature equal to the melting point of the polymer (523 K) at a pressure of 2 MPa. The CNT are coated of nanoparticles copper iodide and BFP, their size is 20-30 nm.

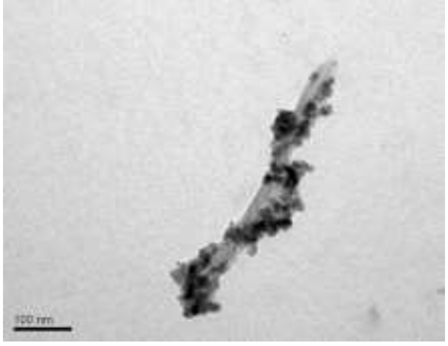

Fig. TEM image of nanocomposites CuI/CNT/BFP–*h*

The introduction of CuI/BNT/PBF in PCTFE leads to an increase of the values of ε', ε'' in 5-7 times in the microwave range, and to the increase of the electrical conductivity values by almost two orders of magnitude. The shift of percolation threshold to a low CuI concentration region compared to a system that does not contain modified components was observed.

However, for the composite CuI/BNT/PBF–*h*, the values of ε', ε'' increased only 2-3 times. This is due to the partial combustion of nanotubes during annealing of composites CNT/BFP.

Selective removal of precious metals by materials with ethylthiocarbamidepropyl groups

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The one-stage template technique [1] and sol-gel synthesis to obtain SBA-15 silica and cover magnetite particles with $\equiv Si(CH_2)_3NHC(S)NHC_2H_5$ groups are proposed. Thus, these approaches open wide (and novel) opportunities for the controlled surface design and porosity. Ratio of reacting components affecting the characteristics of such materials and their sorption properties towards heavy metal ions were analyzed. The synthesized materials were studied by scanning and transmission electron microscopies, Fourier-transform infrared spectroscopy, N_2 adsorption–desorption isotherms, elemental analysis, TGA, and XRD.

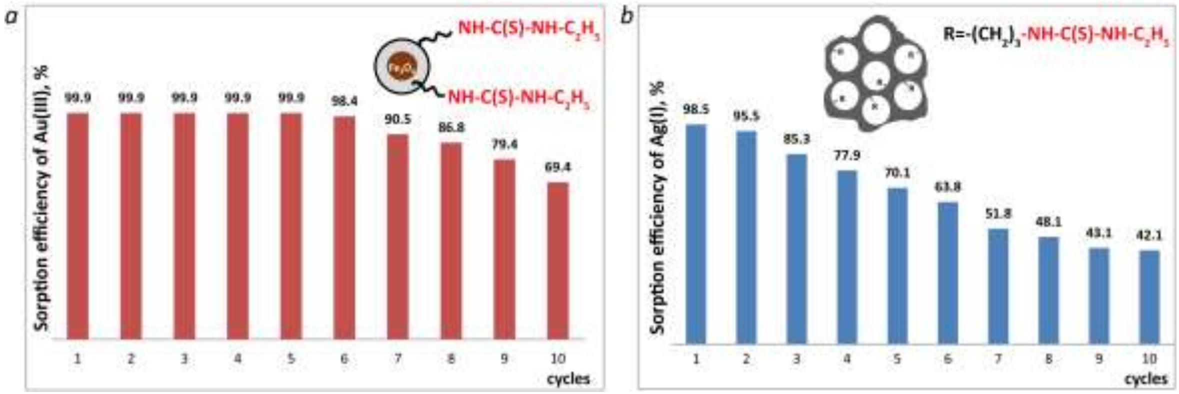

Fig. Concentrating efficiency of Au(III) (*a*) and Ag(I) (*b*) ions from metal ions mixture for the samples containing ethylthiocarbamidepropyl groups

It was shown that the sample with magnetite core and porous silica shell with thiocarbamide groups selectively adsorbs Au(III) ions from water as well as SBA-15 sample with thiourea groups selectively uptakes Ag(I) ions from mixture in the presence of Cu(II), Zn(II), Cd(II), and Pb(II) (Fig.), and they could be regenerated by thiourea solution [2]. So, these materials could be used for concentrating precious metals in acidic medium.

1. G.I.Nazarchuk, I.V.Melnyk, *et al*. J. Colloid. Interface Sci. **389** (2013) 115.
2. I.V.Melnyk, G.I.Nazarchuk, *et al*. Appl. Nanosci. (2018) DOI:10.1007/s13204-018-0761-5.

Corrosion behaviour of high-entropy AlCuCrCoNiFe nanostructured coatings obtained by physical vapour deposition method with cathode arc evaporation (PVD CAE)

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High entropy alloys were shown to demonstrate good corrosion resistance, which is comparable to that of stainless steel [1]. Thus, they are prospective materials to produce protective coatings for different low corrosion resistant metallic materials. It was shown that a physical vapor deposition method with cathode arc evaporation (PVD CAE) is effective in this sense [2].

This work describes corrosion behaviors of the coatings deposited by PVD CAE method from a cathode made of the high-entropy alloy of equiatomic composition AlCuCrCoNiFe. The so-called ‘micro-drop’ regime of evaporation/deposition was used. Thus, according to the SEM data, chemical compositions of the obtained HEA coatings were almost identical to that of the as-cast HEA alloy used as a cathode. The used improved equipment allowed producing relatively thick (~50 μm) homogeneous coatings.

The XRD analysis showed a multi-phase microstructure of the coatings, with two fcc and one bcc phases. TEM observations confirmed that the microstructures of the HEA coatings contain nano-scale and/or ultrafine grains dependently on the regimes of deposition and thermo-physical properties of the substrate material.

Corrosion behaviors of the HEA coatings were analyzed by means of potentiodynamic polarization curves registered in saline solution (3.5% NaCl) [3]. Corrosion resistance of the as-cast AlCuCrCoNiFe HEA and the AlCuCrCoNiFe nanostructured coatings obtained by PVD CAE deposition is observed to be much higher than those for appropriate substrates (low carbon steel and 2024 aluminum alloy) and it is comparable to that of stainless steel [3].

1. Y. Qiu, M. A. Gibson, H.L. Fraser, N. Birbilis, Mater. Sci. Technol. **31** (2015) 1235.
2. V.M. Nadutov, A.V. Proshak, S.Yu. Makarenko, V.Ye. Panarin, M.Ye. Svavilny, Mater. Sci. Eng. Technol. **47** (2016) 272.
3. B.N. Mordyuk, G.I. Prokopenko, M.A. Vasylyev, M.O. Iefimov, Mater. Sci. Eng. A **458** (2007) 253.

Complexing of fullerene C_{60} with some metal lactates: quantum chemical simulation

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Fullerene C_{60} is a quasi-aromatic molecule whose physical and chemical properties have been examined fundamentally. All mechanisms of chemical transformations, synthesized *endo*-fullerenes with various metals, created polymer and composite materials based on fullerene C_{60}, obtained “guest-host” complexes, compiled biological liquids have been studied. However, the C_{60} electron-rich system has been surprising the scientific world up until now.

The ability of fullerene C_{60} to be a ligand in numerous *d*-metals, remaining a strong electron acceptor is of high interest. If a complex compound contains other than C_{60} classic organic or inorganic ligands, we observe a resonant manifestation of certain properties. For example, a complex *Cis*-$[Pt(II)(NH_3)_2Cl_2]@C_{60}$ has increased anti-tumor efficiency, weak resistance of tumor cells to the action of the complex itself, as well as reduced side toxic effects.

Within this framework, we suggest using Mg^{2+} as a strong complexing agent, with lactic acid anion and fullerene C_{60} as ligands.

We have performed a quantum-chemical analysis of possible complexing of $MgLac_2$ with fullerene C_{60}, using MM+, PM3 and Monte-Carlo methods. The optimal structure and absorption spectra of C_{60} with various amounts of $MgLac_2$ on the spherical surface of the latter have been calculated. The constant of complex’s stability has been found to be 68.5 $l \cdot mol^{-1}$ ($k_{korr} \geq 0.98$)

1. S.R. Petrusenko, Ya.O. Vitushinska, V.V. Trachevsky, O.V. Mykhailenko. Ukrainian conference with international participation "Chemistry, Physics and Technology of Surface" and Workshop "Nanostructured biocompatible / bioactive materials", 24-25 May, 2017, Kyiv, p. 124.
2. O.V. Mykhailenko, Yu.I. Prylutskyy, I.V. Komarov, A.V. Strungar, O.O. Mykhailenko. Ukrainian conference with international participation "Chemistry, Physics and Technology of Surface" and Workshop "Nanostructured biocompatible / bioactive materials", 24-25 May, 2017, Kyiv, p. 15.

Synthesis of chitosan microemulsions by membrane emulsification

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Emulsions are usually prepared using homogenizer by generation of turbulent droplet break-up. Some limitations are associated with method of production. These include the droplet size and droplet size distribution cannot easily be controlled, high energy consumption, and poor reproducibility of the product properties [1]. Membrane emulsification characterized with its high ability to control the mean droplet size over a wide range together with the ability to provide a narrow size distribution [2].

In this work water-in-oil (W/O) emulsion has been prepared by method of membrane emulsification. The dispersed phase was Chitosan 0.5% and the continuous phase was sunflower oil containing Tween 80 and oleic acid as emulsifiers. PETF track membrane with pore size 0.1 μm was used for membrane emulsification. The continuous phase was stirred by using magnetic stirrer. The rotational speed was varied from 300 to 500 rpm. The size of particles was studied by Dynamic light scattering method. The DLS measurements were performed using the Malvern Zetasizer Nano instrument (Malvern Instruments Ltd). The Fig. demonstrates that the mean size of produced droplets is approximately 800 nm.

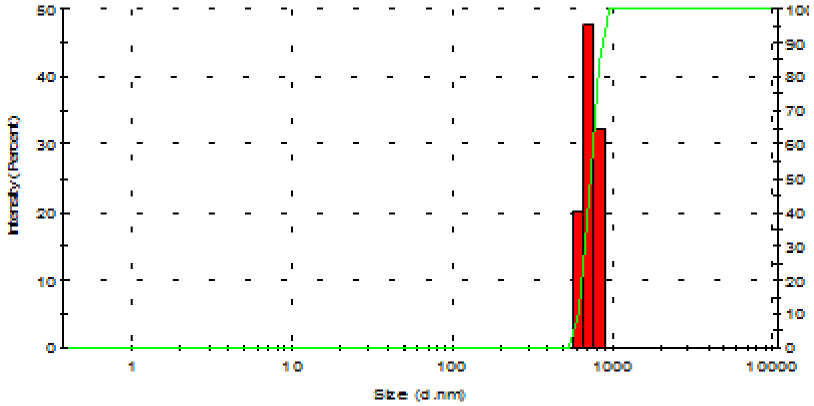

Fig. Curve of size distribution by intensity of chitosan microemulsion

1. E.Piacentini, A. Imbrogno, E. Drioli, L. Giorno, J. Membr. Sci. **459** (2014) 96.
2. J. Santos, G. Vladisavljevič, R. Holdich *et al.*, Chem. Eng. Res. Des. **98** (2015) 59.

Transformation of glycerol and dihydroxyacetone into ethyl lactate and lactic acid on oxide catalysts

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Catalysis and "green" chemistry are the basic driving forces that determine the main directions of development of modern chemistry and chemical production, their key goals are the development of new environmentally friendly processes using renewable raw materials. In this communication the results on obtaining ethyl lactate and lactic acid based on glycerol are presented.

The catalytic experiments were performed using a flow reactor with fixed bed of catalyst (4 cm^3). The reaction temperature of the conversion varied within 140 – 240°C. The products were analyzed by gas chromatography (Chrom-5) and ^{13}C NMR spectroscopy (Bruker Avance 400).

The transformation of dihydroxyacetone in water-ethanol solutions was carried out on amphoteric $ZrO_2 – TiO_2$ oxide (Fig. *a*), the highest selectivity (47 % ethyl lactate and 49 % lactic acid) was obtained on specimens with an atomic ratio Ti/Zr=3 at 140°C with a 100% conversion of dihydroxyacetone [1].

The direct synthesis of ethyl lactate from glycerol was realized due to the oxidation of the reaction mixture of glycerol and ethyl alcohol in an atmosphere of air on a CeO_2/Al_2O_3 catalyst (Fig. *b*). Catalysts are capable of providing ~ 80 % conversion of glycerol with 93 – 95 % selectivity at 230°C and a molar ratio of oxygen : glycerol = 1 : 2 [2].

High-basic $Cu/MgO – ZrO_2$ catalyst is proposed for conversion of alkaline solution of glycerol to sodium lactate (Fig. *c*). This catalyst at 240°C and 2.4 MPa provides 89 % yield of sodium lactate.

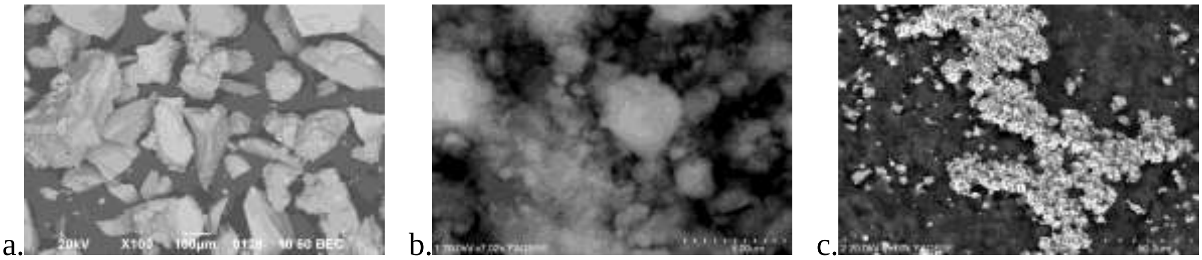
a. b. c.

Fig. SEM images applied catalysts: *a* - $ZrO_2 – TiO_2$; *b* - CeO_2/Al_2O_3; *c* - $Cu/MgO – ZrO_2$

Possible scheme for the reaction with the participation of centers on the surface of the catalysts is discussed.

1. V.V. Brei, A.N. Mylin, Theor. Exp. Chem. **50** (2014) 381.
2. A.M. Mylin, V.V. Brei, Ukr. Chem. Jorn. **82** (2016) 79.

Simulation of molybdenum(VI) oxide interaction with a silica surface

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The process of interaction between molybdenum(VI) oxide and silica surface was simulated using the Restricted Hartree-Fock method (the LCAO approximation). In order to shorten the computing time, the valent basis set SBKJC (Stevens-Basch-Krauss-Jasien-Cundari) was used which required application of the respective effective core potential. The Gibbs free energy (ΔG) values for the considered species were calculated within 298–1100 K temperature interval using the ideal gas, rigid rotor, harmonic normal mode approximations and the pressure P = 101.325 kPa as the sum of electronic energy, zero point energy, and the energy contributions of vibrational, rotational, and translational movements.

$O_{12}Si_{10}(OH)_{16}$ cluster of adamantane-like structure was considered as a model of silica surface. The temperature dependences of the Gibbs free energy of the reaction $O_{12}Si_{10}(OH)_{16} + MoO_3 = O_{12}Si_{10}(OH)_{14}O_2MoO_2 + H_2O$ resulted in the formation of different surface $=MoO_2$ structures was studied. The formation of the most energetically favourable structure (ΔG in the range from -368 to -303 kJ/mol) is shown in Figure for which the energy profile was calculated.

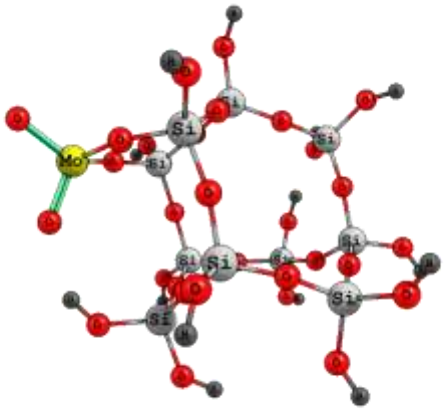

Fig. Optimized geometry of $O_{12}Si_{10}(OH)_{14}O_2MoO_2$ cluster

It has been shown that the reaction begins from the formation of the structure with coordination bond Mo···O (ΔG = -156 kJ/mol at 700 K). Then, a transfer of the proton of Si–OH group to the oxygen atom of MoO_3 molecule (ΔG = -142 kJ/mol and E_{act} = 161 kJ/mol at 700K) takes place. Further rearrangement assumes practically barrier-free (ΔG= +5 kJ/mol at 700 K) rotation around the Mo–O bond. After that, a condensation of the groups Si–OH and Mo–OH with formation of water molecule (ΔG = -2 kJ/mol, E_{act} = 154 kJ/mol at 700 K) occurs. And finally, the water molecule is eliminated and a molybdena-silicate structure $O_{12}Si_{10}(OH)_{14}O_2MoO_2$ is formed (ΔG = -42 kJ/mol at 700 K). The undertaken simulation proves the high temperature interaction between molybdenum(VI) oxide and silica surface which results in the formation of molybdena-silicate structures.

Efficiency of binding of doxorubicin to CNTs and its release during incubation with trypsin

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The aim of the study was to investigate the prospects of multiwall carbon nanotubes (MWCNT) using for the targeted delivery of Doxorubicin (DOX) and the possibility of DOX controlled release from the surface of MWCNT by trypsin. Cytotoxic effect of the resulting materials on tumor cells *in vitro* was investigated also. Colon carcinoma (line HT29) was used as cellular models. The cells were incubated under standard conditions, in 5 % CO_2 in air, 95 % humidity, 37 °C, in DMEM medium supplemented with 10 % fetal bovine serum and 40 mg/ml gentamicin. MWCNTs were obtained by CVD method, purified from catalyst and oxidized in 70 % HNO_3 solution at 100 °C for 4 h. DOX immobilization on the surface of oxidized MWCNT was performed by incubation with solutions of bifunctional water-soluble cross-linking reagent - carbodiimide (N-(3-dimethylaminopropyl)-N-ethylcarbodiimide hydrochloride) and then Doxorubicin-lactose monohydrate. A serine protease, trypsin in stock concentration of 0.25 mg per 100 ml, was used for the release of DOX. It was found that increasing concentration of trypsin from 11 to 20 % leaded to increasing concentration of free DOX from 3.13 to 6.55 μg/ml. A further increasing trypsin concentration to 60 % didn't promote increasing of free DOX. But 66 % trypsin concentration stimulated the release of trypsin again and increased DOX concentration almost in twice, to 11.38 μg/ml. Also, it was found that the simultaneous use of trypsin and MWCNT-DOX significantly increased cytotoxic effect of MWCNT and DOX, comparing with separately activity. So, separately DOX at concentration of 0.05 to 1.0 μg/ml caused dose-dependent decreasing the percentage of living HT29 cells from 7.18 to 45.7 % relative to control. Incubation of MWCNT-DOX with trypsin at concentration of 1.25 to 1.75 μg/ml leaded to dose-dependent decreasing percentage of living cells by 80.9 and 99.8 %, respectively. At the same time incubation with trypsin alone caused to decreasing percentage of living cells by only 34.0–42.0 %.

Morphology of SiO_2/PDMS nanocomposites

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Investigating interfacial interactions of polymers with dispersed solids is important in solving a wide range of issues: from adsorption modification of sorbents to obtaining highly filled polymeric systems. The aim of this study is to determine the effects on morphology of fumed nanosilica A300 by interaction with polydimethylsiloxane PDMS50. The nanosilica/PDMS50 composites were prepared employing impregnation from a hexane solution. The samples were characterized using nitrogen adsorption and DSC methods (Table).

Table. Characteristics of the samples

Code of samples	Polymer content, wt%	ρ_{sample}, g/cm^3	S_{BET}, m^2/g	d_{part}, nm	h_{layer}, nm	d_{part} (h_{layer}), nm	RAF_{int} (wt) (±0.05)	MAF (wt) (±0.05)
A300	-	2.2	297	9.18	-	-	-	-
A300/PDMS50/5	5	2.14	249	11.26	0.17	9.52	-	-
A300/PDMS50/10	10	2.08	221	13.05	0.37	9.92	1.00	0.00
A300/PDMS50/20	20	1.96	171	17.9	0.85	10.88	1.00	0.00
A300/PDMS50/30	30	1.84	106	30.76	1.46	12.10	0.70	0.30
A300/PDMS50/50	50	1.60	51	73.53	1.70	12.58	0.55	0.45
A300/PDMS50/80	80	1.24	3.2	1512.1	2.72	14.62	0.20	0.80

ρ_{sample} – sample density; S_{BET} – specific surface area; d_{part} – BET particle diameter; h_{layer} – thickness of the PDMS layer; $d_{part}(h_{layer})$ = 9.18 + 2 h – particle diameter with counting the thickness of PDMS layer; *MAF* – mobile amorphous fraction, and RAF_{int} – interfacial rigid amorphous fraction.

From the analysis of the data in the table, we concluded to the structure of the studied SiO_2/PDMS nanocomposites, as described by the following scheme:

Fig. Estimated schematic nanoparticles/PDMS distribution for the various PDMS loadings

Up to 20 wt% PDMS, polymer seems to be located exclusively at the interfaces with the particles (RAF_{int}=100 %), whereas for 30 wt% PDMS, and larger, some fraction of the polymer shows mobility contributing to the glass transition, namely, to the MAF.

Application of response surface methodology for optimization of anthocyanin removal from chokeberry extracts by fibrous cation exchanger FIBAN K-1

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In last decades anthocyanins have gathered the attention of the scientific community due to their properties. The range of application of anthocyanins grows as natural colorants in food industry and as antioxidants in medicine, that is why there is growing necessity to obtain these compounds. The adsorption removal of anthocyanins from their extracts is a very promising endeavor. However, nowadays information about optimization of adsorption removal of anthocyanins from extracts is extremely limited.

The objective of this work was to investigate on the relationship between of removal of anthocyanins from chokeberry extracts by fibrous cation exchanger FIBAN K-1and the main parameters affecting it using response surface methodology.

The extract of anthocyanins was prepared from homogenized ripe berries of chokeberry using 0.1 M HCl. The adsorbent was fibrous cation exchanger FIBAN K-1. Adsorption removal of anthocyanins from chokeberry extracts were performed as a function of the time (τ = 30-110 min), temperature (T=283-323 K), adsorbent dosage (m = 2.5-12.5 g/L) and initial concentration of anthocyanins (C = 100-300 mg/L).

The study allowed obtaining the regression equation relating the anthocyanin removal efficiency from chokeberry extracts with the main adsorption parameters:

$$\alpha\ (\%) = 97.91 + 2.72\tau + 5.45T + 2.25m - 1.66C - 1.56Tm + 1.42mC - 1.97\tau^2 - 4.35T^2 - 1.93m^2.$$

For visualization the experimental data we constructed 3D graphics which consider interconnection between different parameters and adsorption removal efficiency of anthocyanins from chokeberry extracts.

Thus, a numerical and graphical optimization procedure was performed to predict the optimal level of the main factors and to obtain the maximum adsorption removal of anthocyanins from chokeberry extracts by fibrous cation exchanger FIBAN K-1.

Investigation of nitrogen-modified graphene by the XPS method

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Introduction of nitrogen atoms to the structure of graphene is a promising method for modifying their physical and chemical properties [1]. This makes it possible to obtain high catalytic characteristics of graphene without the use of noble metals [2].

In this paper, the results of the modification of plasma-chemical synthesis of graphene by nitrogen atoms are investigated by the method of X-ray photoelectron spectroscopy (XPS). The appearance of a transparent in the visible range of the carbon phase is recorded.

According to the XPS, the C1*s*-line of samples, along with the contribution of sp^2C-sp^2C (E_b = 284.8 eV), is characteristic of graphene, contains a component of E_b= 286.4 eV, which is associated with N-sp^3C bonded nitrogen-modified graphene [1-2]. The phase is not a graphene oxide, since components that correspond to C-O and C=O bonds are absent in the C1*s* spectra.

On the spectra of the N1*s* line, in addition to the four components (398.5, 399.8, 401.6 and 402.7 eV) [1-2] characteristic of nitrogen-modified graphene components with E_b = 405.6 and 406.7 eV are present.

The mechanisms of appearance of a new phase and adsorption centers are discussed. It is shown that the XPS method can be used as a feedback element to optimize the synthesis parameters.

1. A.L.M. Reddy, A. Srivastava, S.R. Gowda, H. Gullapalli, M. Dubey, P.M. Ajayan, ACS NANO **4** (2010) 6337.
2. Y.P. Zhu, C. Guo, Y. Zheng, and S. Qiao, Acc. Chem. Res. **50** (2017) 915.

Synthesis and mass spectrometric investigation of lanthanide complexes with polydentate carbacylamidophosphates (CAPh ligands)

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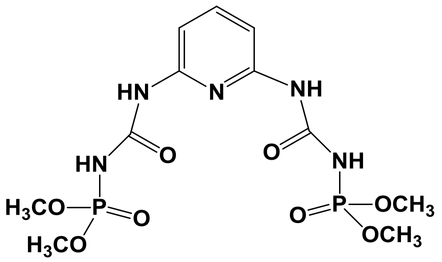
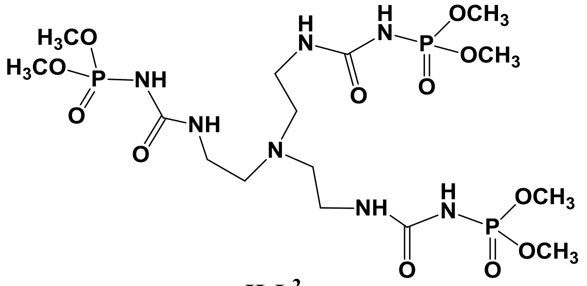
Coordination compounds of lanthanides with polydentate β-diketones and their derivatives lately have attracted especial attention due to the advancement of technology MOLED (metal organic light emitting devices), as well as the possibility of using such compounds in biomedical research and as contrast reagents for NMR tomography studies. From this standpoint, the selection of appropriate ligands, which are effective sensitizers of lanthanide luminescence and can form thermodynamically stable complexes, is especially important.

Carbacylamidophosphates (CAPh ligands) of general formula $(R^1)C(O)NHP(O)(R^2)$ are structural analogues of β-diketones, which can serve as an antenna providing more efficient energy transfer to the lanthanide ion followed by Ln(III) luminescence.



H_2L^1



H_3L^2

Two new polydentate CAPh ligands (H_2L^1, H_3L^2) have been synthesized. The lanthanide coordination compounds of general formula $Na[LnL^1_2]$, $[LnL^2]$, $[Ln(H_2L^2)](NO_3)_2$, $[Ln(HL^2)]NO_3$ (where Ln = La, Lu, Tb) were obtained and characterized by method of LDI mass spectrometry. This method allows to get information about the composition of complex, to estimate stability of the complex particle and the nature of intramolecular bonds due to analysis of the fragments and associates. The mass spectra of all compounds under consideration do not content the molecular ion peak. This testifies that the loss of one electron by complex molecule results in destruction of excited molecular ion and formation of positively charged ion-fragments which intensity probably corresponds to that of molecular ions in mass spectra.

Magnetically sensitive nanocomposites for targeted transport of Gemcitabine anticancer drug

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The nanotechnology of modification of surface of magnetically controlled nanostructures with use of anticancer drug for chemotherapeutic action is developed. This anticancer drug – Gemcitabine (GC) is used to inhibit of hepatocellular carcinoma (HCC) and intrahepatic cholinchocarcinoma (IHCC) tumors.

Nanocomposites which are based on one-domain magnetite – Fe_3O_4/C are synthesized. The carbonization of the surface of magnetite is carried out with the use of an organic substance – polygel CS (Carbomer 934). The structure and functional composition of their surface are investigated by methods of X-ray diffraction analysis, UV-spectroscopy, IR-Fourier spectroscopy.

The processes of adsorption of Gemcitabine on the surface of magnetite and synthesized nanocomposites of Fe_3O_4/C are studied. Adsorption of Gemcitabine is A = 25-30 mg/g (C_0 = 0.8 mg/ml, g = 30 mg, V = 5 ml). The number of GC on the surface is determined by spectrophotometric method at λ=268 nm (Fig.).

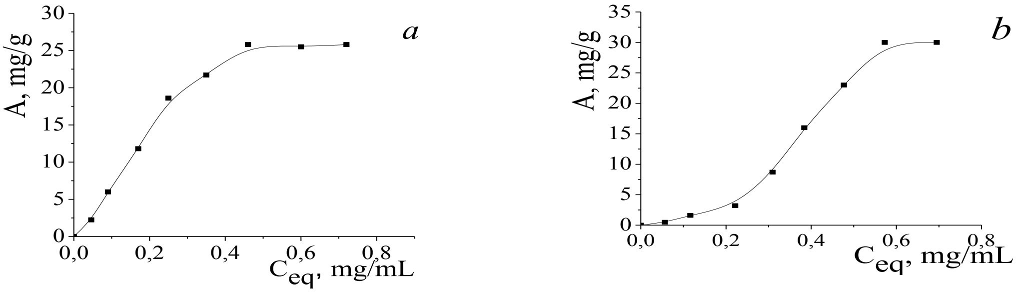

Fig. Isotherms of adsorption of Gemcitabine on the surface of Fe_3O_4 (*a*) and Fe_3O_4/C (*b*)

The results obtained form the basis for further research on the use of magnetically sensitive nanocomposites for targeted delivery of drugs, hyperthermic therapy and magnetic resonance diagnostics.

1. M. Parsian, G. Unsoy, P. Mutlu *et al*., Eur. J. Pharmacol. **784** (2016) 121.
2. R.C. Popescu, E. Andronescu, B.S. Vasile *et al*., Molecules. **22** (2017) 1080.

Complex X-ray diffraction and thermal analysis of bentonite clays

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Adsorptive and ion-exchange properties of bentonite clays are determined by the properties of minerals of the montmorillonite group, which are the main components of the clays. These minerals belong to three-layered silicates with a swelling crystalline lattice, having the general formula $(Na,Ca)_{0.33}(Al,Mg)_2(Si_4O_{10})(OH)_2 \cdot nH_2O$. The peculiarity of their structure is the filling of inter-pack space with water molecules and metal cations capable of exchange with the external environment. They are microcrystalline and highly disperse materials that is, they can be called nanomaterials. Bentonite clays are used in industry, agriculture, medicine. At present, the possibilities of their modification for use in medicine and cosmetics are expanding. Knowledge of the phase composition of clays is necessary for their practical application. X-ray diffraction and thermal analysis are the main methods for identification of the phase composition of clays [1].

Three series of clays are investigated, such as clays of known phase composition, food and cosmetic clays. By the XRD method the minerals of the montmorillonite group, the accompanying minerals were identified in food and cosmetic clays using dry and swollen in water and glycerol samples of clays (Fig. 1). The heterogeneity of the phase composition is confirmed by thermal analysis data (Fig. 2). The presence of kaolinite, calcite, quartz, gypsum, mica in bentonite clays was also confirmed by X-ray diffraction when using clay samples annealed at the temperatures of the characteristic thermal effects, that were observed on the derivatograms. The content of these minerals varied considerably in the test samples.

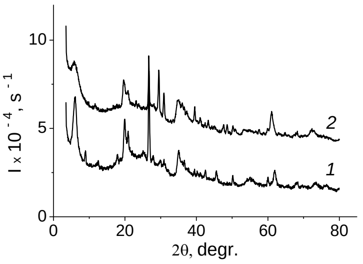

Fig. 1. XRD patterns of montmorillonite (*1*), cosmetic clay Rassul (*2*)

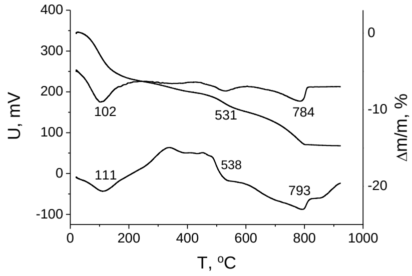

Fig. 2. Derivatogram of food blue clay

1. V.A. Frank-Kamenetsky, X-ray analysis of the main types of rock-forming minerals (layered and frame silicates), L.: Nedra, 1983 (in Russian).

Georgian natural zeolites for treatment of sewage waters

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One of the steps in the various technological schemes for sewage water treatment is its filtration. The vast majority of the filtering materials are synthetic while inexpensive, widespread, easily available and effective filtering materials such as mineral-zeolites were vainly left beyond attention.

Zeolites, as cationic type ion exchangers, extract heavy metal cations from water and compared to synthetic resins they have higher selectivity to cesium and strontium ions.

The purpose of this work is to investigate the feasibility of application of Georgian natural zeolites (Hekordzula and Botanikuri regions) for decreasing mineralization of sewage waters and extracting undesired toxic impurities by improving adsorption activity of sorbent.

In order to achieve the above goal, combined filtration column (5×20 cm) filled with the following adsorbents was prepared: 1st layer (5 cm) - clinoptilolite (granules of 2-2.5 mm) washed with 1 N HCl and heated at 200-250°C; 2nd layer (5 cm) lomontite (granules – 1.5-2 mm) prepared in the same way; 3rd layer (5 cm) – natural clinoptilolite (0.5-1 mm granules); 4th layer (5 cm) - quartz sand washed with 1 N HCl and heated at temperatures of 200°C.

To prepare granules of hydrogen forms of clinoptilolite and lomontite containing about 90% crystalline phases were placed in a flask and 1 N HCl was added to it in the amount of 10 volume of the solution per volume of the sorbent. The flask connected to a backflow condenser was placed in a sand bath and boiled the content of the flask for 4 hours. According to this procedure, 200 cm^3 of sorbent (granules of 2.5-0.5 mm) was treated. The prepared sorbent was loaded into a glass column with an internal diameter of 5 cm. 4 L of the wastewater sample flew through the column at a speed of 5 ml/min. It has been established that the use of hydrogen forms of lomontite and clinoptilolite significantly improves cationic composition of the filtrate. Comparison of the data proves that content of Mg^{2+}, Ca^{2+}, SO_4^{2-} and Cl^- ions decreases about 40%. Significantly decreases the content of such undesirable ions as Pb^{2+} Fe^{2+}, Fe^{3+} , Sr^{2+}, Mn^{2+} , Zn^{2+}, Cu^{2+}, Co^{2+}, and Ni^{2+} (about 100-50 %).

Thus, the above natural zeolites might be used as filter materials in the field of environmental protection and be relevant for both practical and economical point of views.

Physicochemical properties of clay adsorbents for oral administration

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Usage of native clays as enterosorbents is becoming increasingly popular due to the non-toxic properties, maintenance of structural integrity of the gut mucosal barrier and intestinal microflora, easy evacuation from the intestine, sorption properties, when applied perorally.

Novel clay-containing composites have been developed expanding the scope of clays application in medicine and cosmetics considerably. However, naturally-sourced materials are distinguished by structural and chemical heterogeneity. Therefore, for the further bio-medical application, a thorough study of their physical and chemical properties is required. In this work the XRD analysis, FTIR and TPD-MS, iodometry, sorption of dyes and water-glycerine mixture were used. Clays, investigated within this work were classified in regards to their interaction with dyes and water-glycerine mixture, also by FTIR and XRD (Fig.) analysis. All clays show a low affinity to iodine. A TPD-MS results show that the chemisorption of water from the clay surface is strongly depends on structure of the surface and the type and concentration of surface hydroxyls.

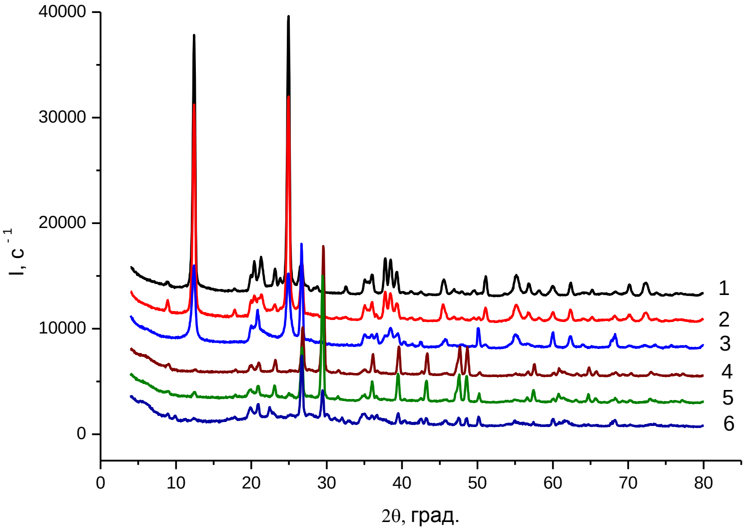

Fig. XRD graphs of clays: kaolin (*1*), white-blue clay (*2*), light-blue clay (*3*), bentonite (*4*), green clay(*5*), blue clay (*6*)

Preparation of composite materials with nanosilica, kaolin clays, and pius pollen for cosmetic purposes

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Currently, one of topical directions is the creation of composite materials with bioactive substance (BAS) that allows one to regulate the kinetics of BAS release. From this point of view, systems consisting of biodegradable polymers and clay materials are promising. Varying the composition of such systems will make it possible to regulate the process more effectively.

The purpose of this work was to create a composition of highly disperse (HDS) and laminated (kaolin clays) materials appropriate as carriers of BAS. The different nature of interactions of BAS with highly disperse constituent and clays could favour to solve the release control problem.

In the preparation of composites based on biopolymers and clays used as carriers of BAS, mostly highly dispersed clays are applied.

In this paper, the effect of dispersing kaolin clay / A-300 and kaolin clay/pinus pollen/A-300 systems with knife mills was studied.

The particle size distribution was determined using dynamic light scattering with Zetasizer-3 and Zetasizer NanoZS (Malvern Instruments, UK). A 0.005% aqueous suspension of the preparations was examined that was additionally subjected to ultrasound treatment prior to measure the deaggregation of the secondary particles.

The combination of kaolin clay with A-300 in a composite material allows us to reduce the diameter of particles by 1.5-2.5 times. Composite materials were used as components of cosmetics (shampoos, toothpastes).

Network characteristic of films with styrene-acrylic polymer and dispersion of silver nanoparticles

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The interest to the materials based on polymers and nanoparticles of semiconductors or precious metals is linked to their possibility to provide specific or even unique properties to the materials such as durability, thermal and chemical inertness. Therefore, these films and coating can be used in various industries. However, to date there is no integrated practice of a full investigation of the structure polymer films with inorganic nanoparticles.

The aim of current research is to analyze and compare polymer films based on styrene-acrylic polymer (Lakritex 430) and dispersion of silver nanoparticles (Ag^0) synthesized in aqua solution using different precursors (Sodium citrate, Ascorbic Acid, Trilon B, Tannin), with the theories of gel network formation and swelling. Using equilibrium swelling method crosslinking density (*j*,%), sol fraction (*S*,%), and swelling degree (*a*,%) in nanocomposites films were calculated.

Table. Network characteristic of styrene-acrylic polymer films with silver nanoparticles

	Lakritex 430	Lakritex 430 Silver Sodium citrate	Lakritex 430 Silver Ascorbic Acid	Lakritex 430 Silver Trilon B	Lakritex 430 Silver Tannin
S, %	12.9	2.02	14.7	21.59	43.08
a, %	14.05	22.3	22.6	35.5	33.22
j %	6.04	8.02	6.08	4.1	2

Table shows, that polymer film with silver nanoparticles synthesized with sodium citrate has higher concentration of double bonds; so the latter will exhibit higher density of crosslinking at equal degrees of conversion and will form tighter networks. Such polymer compositions and polymer films lead to the improved mechanical properties of individual polymers.

Polymer films with silver nanoparticles synthesized in Trilon B and tannin diminish crosslinking density. Such films are dissolved in solvents more quickly which means that this nanopolymer composition not form crosslinking structure. The differences in the crosslinking behavior of the four nanopolymer films must be due to the different chemical interaction between spacer group of acrylates and reactive groups of precursors.

Structure and magnetic properties of Ni-C hybrid nanofilms

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Magnetron sputtering allows obtaining the nanocolumnar arrays of various materials. Hybrid nanocolumnar structures of "core/shell" type nanoclusters, for example magnetic metal covered with carbon are the objects of special interest. Structure and properties of such materials are studied intensively because of their high potential applications [1, 2].

The purpose of this research is to study the structure and magnetic properties of hybrid Ni-C films synthesized at low temperature magnetron deposition of nickel-carbon clusters. Two groups of films were grown in which C/Ni-ratios were: 30/70 – I group; 40/60 – II group. Film thicknesses were up to 100 nm. The growth time of the films varied in limits of 10 s up to 10 min.

The nanoscale clusters of sputtering material generated in plasma are deposited onto substrate surface. Formation of clusters in plasma is caused by high enough pressure of buffer gas and low power of magnetron plasma. X-ray diffraction patterns of I group films shows the presence only the reflexes corresponding to the FCC-lattice of nickel. Presence of carbon in structure of films indicates existence of a carbon cover around of nickel nanocrystallites as it is shown in works [3].

II group films (C/Ni=40/60) at high substrate temperature demonstrate nickel FCC-phase. At substrate temperatures ≤ 150°C reflexes of a new phase which has been identified by us as NiO are registered. It is possible, that the increase in concentration of carbon in Ni-C films leads to change of carbon structure covering the nickel nanocrystallite. The increase in concentration of carbon in Ni-C nanoclusters conduces to the following carbon covers around metal nanocrystallites are not closed, and consist of imperfect bent fragments with pores. The increasing in substrate temperature leads to increase in degree of orderliness of the bent carbon fragments and provides protection of Ni-crystallites against oxidation.

Magnetic measurements have shown that I group samples have ferromagnetic properties at deposition on a cold substrate, while for II group ferromagnetism arises at achievement some critical temperature of substrate ~ 80°C.

1. El Mel A., Gautron E., *et al*. CARBON. **49** (2011) 4595.
2. Shalaev R, Prudnikov A, Yoo S, Phys. Status Solidi A. **209** (2012) 2300.
3. Sacanna S, Rossi L and Pine D. J. Am Chem. Soc. **134** (2012) 6112.

Preparation and properties of biodegradable composite materials based on polyvinyl alcohol and starch

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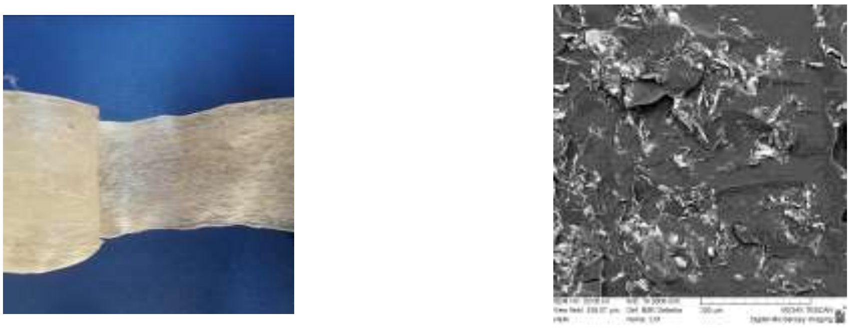
The development of biodegradable composite polymers is considered a solution for solid waste storage problems. Polyvinyl alcohol (PVA) is a biodegradable synthetic polymer, non-toxic, soluble in water. PVA exhibits excellent mechanical properties and is compatible with the starch. But PVA is high-cost material; hence a potential solution to decrease the cost of packaging and to enhance the hydrophobicity lies in preparing of composites with cheaper fillers, such as starch and cellulose with addition of hydrophobizing components.

In this presentation, the preparation methods and properties of PVA-starch and PVA-starch-wood flour completely biodegradable composites are presented. The preparation process of powder mixture is following: PVA powder, modified potato starch, plastificators and polydimethylsiloxane are mixing in blender at the temperature 90±5 °C, mixing time 30 minutes, speeds of rotors 300 rpm. The melting of blends and band preparation was performed using a Haake Rheocord 90 extruder in the following conditions: temperature of 170 – 180 °C, band thickness of 0.5 mm (Fig. *a*).

For composite properties modification the corn starch and wood flour (Fig. *b*) were introduced into initial mixture. The results show that the addition of starch and wood flour into blends leads to decrease both tensile strength and elongation at break of so prepared composition.



a *b*

Fig. Composite band PVA-starch-wood flour (*a*); SEM-picture of this band structure (*b*)

Dynamics of silver and copper ions release from bactericidal textiles modified by Ag and Ag/Cu nanoparticles in an aqueous medium

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Nanosized particles (NPs) of silver and copper, which are widely used in antibacterial tissues, cosmetics, water filters, for biomedical applications, and others are an alternative to bactericidal antibiotics [1-3 and references therein]. Silver and its compounds are ionized in the presence of water, biological fluids, or exudates of wounds. Both NPs and ions released from them are toxic for bacteria. The real contribution of NPs and the corresponding ions in the bacterial destruction is unexplained till now. In this work the amount of released ions from the cotton tissue (ct) surfaces modified by NPs, namely Ag-ct and Ag/Cu-ct has been studied. Tissues were kept in water for 24 hours, after which the amount of desorbed ions was measured. These procedures were repeated every 24 hours for three days. For comparison, the same experiments were carried out for tissues modified with Ag^+ and Cu^{2+} ions in the same amount. The dynamics of the release of silver ions in % from Ag-ct for 3 cycles is 40, 7.7 and 0.7, respectively (for fabrics modified with Ag^+ ions, for 3 cycles this amounts are 8, 1 and 0.1%). From the Ag/Cu-ct surface, the amount of silver ions released from the surface in the first cycle is less than 27% compared to Ag-ct, which may indicate that part of the Ag NPs is not included in the BMNPs. In case of Ag/Cu-ct, for 3 contact cycles 13, 1 and 0.1% ions of silver in washout water respectively were obtained. After 24 hours, 17% Cu^{2+} from the surface of Ag/Cu-ct are released, in the subsequent washout cycles, copper ions in water were not detected. The obtained results explain the high bactericidal activity of modified cotton textiles precisely in the first day of their use for disinfecting.

1. C. Levard *et al.*, Environ. Sci. Technol. **47** (2015) 5738.
2. A. Tlili *et al.*, Nanotoxicology. **10** (2016) 728.
3. A.M. Eremenko, I.S. Petrik, A.V. Rudenko *et al.*, Nanoscale Res. Lett. **11** (2016) 28.

Green phosphor Y_2O_3 Tb^{3+} nanostructured powders prepared by the combustion method

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Phosphors are technologically important materials for display applications such as fluorescent lamps, display monitors FEDs *etc*. The phosphor materials fabricated in the form of nanostructures made of rare-earth ion-doped oxides would be better for luminescent applications because they exhibit interesting physical properties and increased luminescence efficiencies, which are different from those of their bulk counterparts. Therefore, they possess diverse potential applications in nanoscale electronics and advanced photonics [1].

Nanostructured powders of yttrium oxide doped with terbium Y_2O_3:Tb^{3+} (green phosphor) were synthesized by the thermochemical method (combustion) under the conditions of oxidation–reduction of nitrate salts of yttrium and terbium in the presence of urea and hexamethylenetetramine as a complex fuel. The combustion at the temperature of ignition 350°C and calcination 650°C provides the powders preparation with the average size particles 102 nm. The products were characterized by X-ray diffraction, scanning electron microscopy, and IR-spectroscopy.

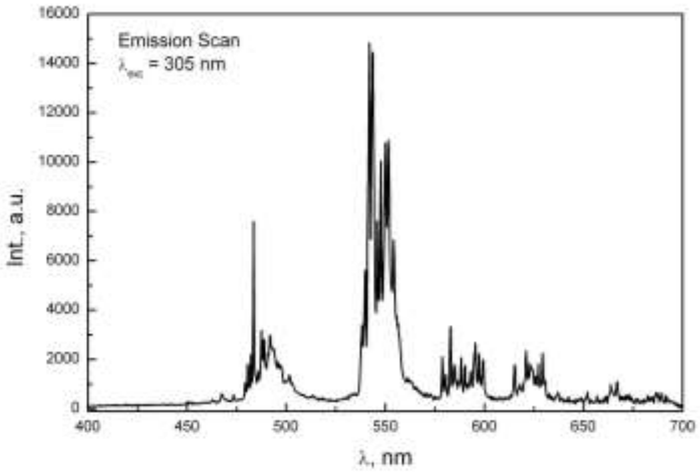

Fig. Luminescent spectra Y_2O_3:Tb^{3+}at excitation of 305 nm

The doping of yttrium oxide by terbium ions causes multiband luminescence with bands in green region (537–563 nm) at excitation wavelength of 305 nm (Fig.).

1. R. Withnall, M.I. Martinez-Rubio, G.R. Fern *et al.* J. Opt. A: Pure Appl. Opt. **5** (2003) S81.

Calculation of pourbaix diagrams for FeCrAl system within the framework of Accident Tolerant Fuels (ATF) concept

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Conventional Zr-based fuel cladding with UO_2 fuel has dominated light water reactors (LWR) for decades, however, the beyond design basis accident (BDBA) in three units at the Fukushima Daiichi power plant in March 2011 has spawned a search for materials that can provide larger safety margins and potentially avoid severe core degradation. Finding a fuel configuration that can better tolerate the loss of coolant than Zr-based alloys has become an important task for the international community.

Nickel is undesirable from a neutronics perspective and chromia-forming Fe–Cr alloys require very high (~25%) Cr contents for steam oxidation resistance at 1200°C. An extensive effort has been conducted to evaluate Fe-Cr-Al alloy properties and develop an optimized composition for the ATF application. The Fe-Cr-Al alloy class has been widely used with success in many industries where high temperature oxidation resistance is needed including water-vapor containing environments in fossil fuel energy plants.

Fe-Cr-Al alloys consist of nominally 10–15 wt% chromium and 3–6 wt% aluminum dissolved in a body-centered-cubic (BCC) iron lattice, which stabilize the BCC structure to the melting point of the material (~1500°C). These alloys possess high-temperature strength and excellent oxidation resistance.

The Pourbaix diagrams allows to determine the possibility of corrosion with hidrogen or oxygen depolarization.

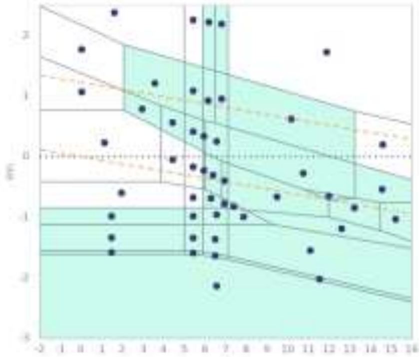

Fig. Pourbaix diagram for Fe(80%)-Cr(15%)-Al(5%) [2]

1. S.J. Zinkle *et al.*, J. Nucl. Mater. **448** (2014) 1.
2. Materials Project. https://materialsproject.org/

Spectroscopic study of products of photoinduced reaction between gold and tryptophan

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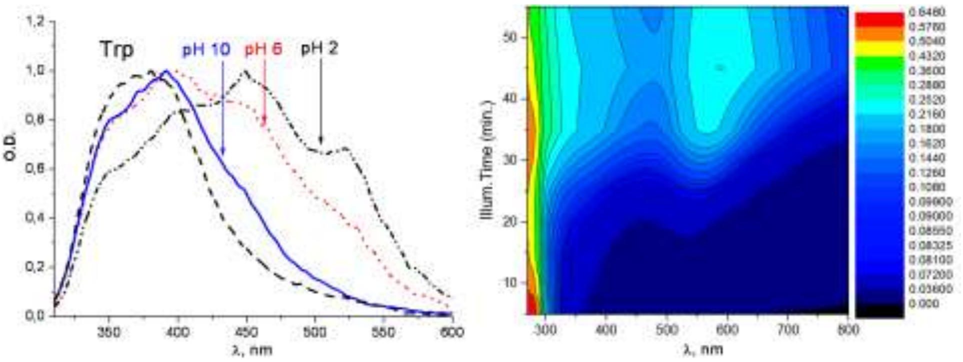
Nanosized gold (Au NPs) has a great potential for targeting, imaging and treatment of cancer. The essential amino acid tryptophan (Trp) is appropriate for synthesis of gold nanoparticles resulting in their toxicity decrease. The reduction of Au^{3+} ions by Trp can occur in the process of chemical, as well as photochemical reaction, initiated by UV light. In the present work we provide the spectroscopic study of products of photoinduced reaction between gold and tryptophan with the use of mercury lamp DRT-125 as UV light source.

Time-dependent absorption profiles of Au/Trp system were not the same when reaction between metal and amino acid occurred at different pH of initial solution of Trp. The oxidation products of tryptophan used in cationic, neutral, and anionic forms, that correspond to pH = 2, 6, and 10 respectively, appeared in absorption spectra as bands with different shapes and location of their maxima. Also the acidity influenced greatly on reaction rate. In particular, the absorption band of localized surface plasmon resonance of gold appeared after 20 min for pH = 6 at 20°C (λ_{max} = 570 nm), while the formation of Au NPs in alkaline medium required day(s) (λ_{max} = 525 nm). Fluorescence spectra indicated formation of new substances with emission band maxima located at 450 and 520 nm, shifted greatly compare to λ_{em} = 380 nm for Trp (Fig.).



a *b*

Fig. Fluorescence spectra of product of reaction in Au/Trp system at different initial pH of medium, λ_{ex} = 280 nm (*a*) and time-dependent absorption spectra in Au/Trp system under UV illumination at initial pH = 6 (*b*)

Electrophysical characteristics of polymer nanocomposites based on barium hexaferrite modified copper iodide

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The protection of the person from electromagnetic radiation is actual problem, which has grown due to the increase in the number of electronic products and devices in the means of wireless communication, local area networks and other communication equipment. Considerable interest was directed to materials that absorb electromagnetic radiation with greater efficiency over a wide range of frequencies.

To create such materials, nanocomposites have been synthesized on a basis of barium hexaferrite. Hexaferrite ($BaFe_{12}O_{19}$) was synthesized using the modified sol-gel technique. The starting materials such as iron nitrate, barium nitrate, citric acid, and ammonia were used. The citric acid was used as a chelating agent. After the gel formation, the temperature of the hot plate was increased to about 523 K for further ignite. The prepared powder was ground and the heat treatment was carried at 1023 K for 5 hours (Fig. 1). The samples $BaFe_{12}O_{19}$ were prepared by a chemical method during the course of release of CuI from an aqueous solution in the presence of $BaFe_{12}O_{19}$. The samples of system CuI/$BaFe_{12}O_{19}$–polychlorotrifluoroethylene (PCTFE) was compacted at the temperature equal to the melting point of the polymer at a pressure of 2 MPa.

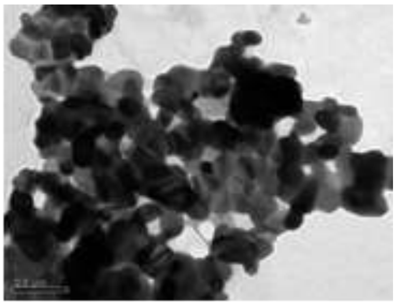

Fig. 1. TEM image of $BaFe_{12}O_{19}$

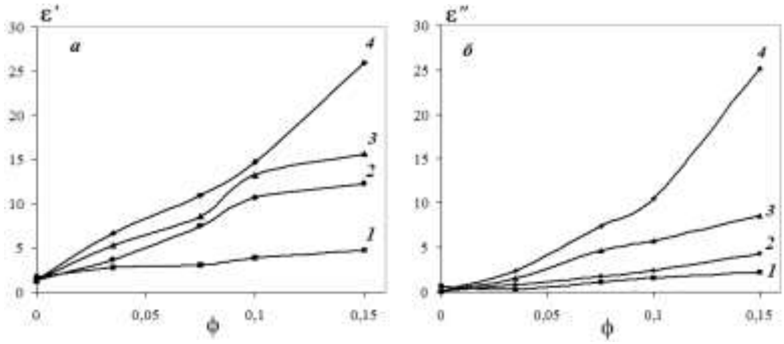

Fig. 2. Dependence of ε'(a) and ε'' (b) at a frequency of 9 GHz polymer nanocomposites by volume content (ϕ) of copper iodide in systems: *1* – CuI–PCTFE, *2* – 0.32CuI/$BaFe_{12}O_{19}$, *3* – 0.32CuI/BFP, *4* – 0.39CuI/$BaFe_{12}O_{19}$

The introduction of CuI/$BaFe_{12}O_{19}$ in PCTFE leads to a significant increase in the values of ε 'and ε'' (Fig. 2).

Biological synthesis of Ag_2S nanoparticles and study their antibacterial properties

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Silver sulfide (Ag_2S) nanoparticles possess unique semiconducting, optical, and electrical properties and are highly stable. They are broadly used in solar cell batteries, thermoelectric sensors, biosensors [1]. An alternative approach to nanoparticle production under mild conditions can be a biotechnological process with biological matrices. Common requirements imposed on nanoparticles include reproducibility, narrow shape and size distribution, stability, a simple protocol, and the absence of toxic substances. The purpose of this study is to develop a new eco-friendly method for biosynthesis of Ag_2S nanoparticles using *Pleurotus ostreatus* as biological matrix and to estimate their antibacterial properties.

Cultivation of *P. ostreatus* was carried out in 100 mL flask with 50 mL of Glucose Yeast Peptone liquid medium under 28°C for 10 days. 0.025 M solutions of $AgNO_3$ and Na_2S were poured into the flasks with fungal mycelium in order to synthesize Ag_2S. Absorption spectra of obtained nanoparticles were measured using a spectrophotometer Specord UV-VIS. Characterization of Ag_2S nanoparticles was carried out using electron microscope JEOL JEM-2100F. *Escherichia coli* and *Bacillus thurengensis* were used as model organisms to test the antibacterial activity of Ag_2S nanoparticles at the following concentrations: 0.3, 0.6, 1, 1.5, 3 mg/mL. Paper discs were soaked with different concentrations of Ag_2S and placed on the surface of Petri dishes with bacterial strains. The incubation was carried out in a thermostat at a temperature of 37°C for 24 hours. Measurement of lysis zones of *E. coli* and *B. thurengensis* was performed using a software Image J (1.38 d). It was found that absorption maxima of Ag_2S nanoparticles corresponded to 315 and 470 nm. Obtained nanoparticles have a size within 20-25 nm. It was found that *E. coli* and *B. thurengensis* strains are sensitive to Ag_2S quantum dots. Inhibition of bacterial growth was observed under 1.5-3 mg/mL of these nanoparticles. Thus Ag_2S quantum dots could be used as nontoxic labels or nanocarriers in cell biology studies.

1. S.I. Sadovnikov, Y.V. Kuznetsova, A.A. Rempel, Nano-Structures & Nano-Objects. **7** (2016) 81.

Nanostructured zirconium silicates as supports of catalysts for dehydrogenation of propane into propylene

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The process of propane dehydrogenation (DHP) to propylene - valuable raw material for the chemical industry is currently being extensively developed. The commercially used DHP catalysts consist of Cr_2O_3 or Pi-Sn, supported on Al_2O_3. They are respectively toxic or expensive, lose activity after numerous regenerations in 1-3 years of work and are subject to replacement. In this work, vanadium oxide supported on a differently structured spherically granulated zirconium silicates, which were obtained by sol-gel synthesis from available salts of elements using the technology of coagulation in drop, were investigated as catalysts for the process of DHP.

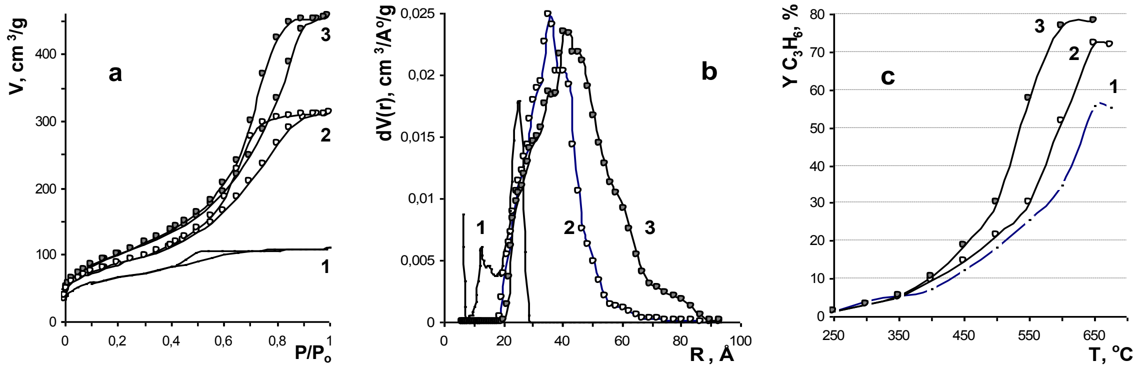

Fig. The isotherms of low-temperature nitrogen adsorption (*a*), the distribution of pores by the radius dimensions (*b*) and the yield of propylene during DHP in a mixture containing 7 vol.% of C_3H_8 in argon (*c*) on catalysts of 10% V_2O_5/0.6Zr-Si-H, obtained after calcination at 450°C - *1*; preliminary subjected by HTT at 250°C for 5 h - *2*; additionally decanted with alcohol - *3*

It was found that the modification of zirconium-silica xerogel by titanium dioxide contributes to the preservation of the specific surface area of mixed oxide, the forming more isolated active sites during application of vanadium oxide and the obtaining more high propylene yield in the DHP.

It was shown that the supporting of vanadium oxide on the zirconium silicate hydrogel and its subsequent hydrothermal treatment (HTT) and decantation with alcohol makes it possible to obtain catalysts with an ordered developed mesoporous structure and increased values of the specific surface, volume and diameter of the mesopores. In the process of dehydrogenation of propane on such catalysts, the yield of propylene is obtained much larger and at lower temperatures than on an industrial Pt catalyst.

pH-sensing properties of transparent silica film with chemically immobilized alizarin yellow

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Design of pH-sensitive materials with acid-base indicators incorporated into the proton permeable silica matrix has attracted considerable interest over the last years due to their potential application in chemistry, biology and medicine. Covalent bonding of pH-sensitive substance to silica surface is attractive alternative to impregnation or encapsulation within silica framework as assures firm retention of sensor moieties in the surface layer and provides direct contact of grafted pH indicator with analyte in the external environment. However, chemical immobilization of pH indicator on substrate proceeds thorough involving of its functional groups in covalent bonding and can lead to the lost of functionality and substantial changes in protolytic properties. So we focused on preparation of optically transparent silica film with covalently bonded alizarin yellow (AY) and comparative study of its protolytic properties.

Optically transparent thin film of pH-sensitive organosilica was fabricated onto glass substrate by casting technique. The sol-gel solution was prepared by hydrolysis and co-condensation of (3-aminopropyl)triethoxysilane and synthesized dye-containing silane in water-ethanol medium using hydrochloric acid as a catalyst. Organosilica film was characterized by Fourier transform infrared spectroscopy and low-temperature nitrogen adsorption-desorption.

The acid ionization constants K_a of individual and chemically immobilized AY were evaluated using ultraviolet-visible absorption spectroscopy measurements. It was found that the pK_a value of AY decreases from 10.9 to 5.5 as a result of covalent bonding to silica surface. Protolytic properties of surface AY-containing groups were studied in the presence of β-cyclodextrin to confirm their potential ability to form host–guest inclusion complexes. In accordance with the obtained results, phenolic hydroxyl group of AY becomes more acidic in the presence of oligosaccharide and dissociates in a less alkaline pH range (pK_a decreases from 10.9 to 10.5). Contrariwise, the ionization of phenolic hydroxyl group in AY-containing silica film takes place at higher pH values at addition of β-cyclodextrin (pK_a increases from 5.5 to 5.9).

Synthesized optically transparent organosilica film exhibits quick pH-responsive color change, reversibility as well as good stability at multiple immersions in aqueous solutions with acidic and neutral pH values.

Silica-based laevomycetin controlled release nanocomposite

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Creation of composites containing carrier-bound antibiotics (via adsorption interactions) as bioactive compound is one of the promising routes of such systems efficiency raising [1]. Wherein rapid drug release (40-60%) during 10-20 min for antibiotics is optimum curve shape for control release dosage form. This prosess is followed by diminishing of drug release during 2-3 hours. Therefore, compacted silica, applying as carrier, is one of the drug manufacturing operations imperetives [2]. Required compaction value can be achieved by silica impregnation from antibiotic (laevomycetin) alcohol solution due to given in advanced concentrations of active compound, solvent and silica, consequently.

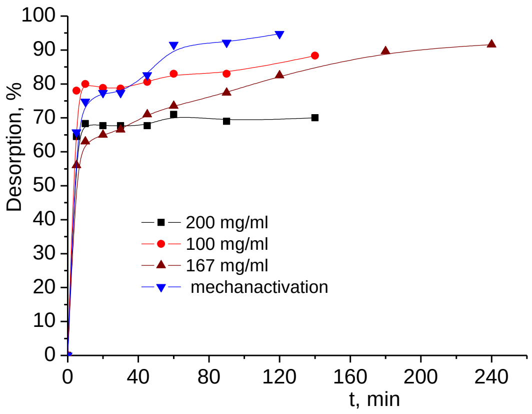

Fig. Dependence of laevomycetin desorption value (%) on time (min)

Figure illustrates desorption curves for samples with different tapped density (C_d) and methods of preparation. First two samples ($C_d = 100$ and 200 mg/cm^3) were prepared under the conditions of quick solvent evaporation, the third one ($C_d = 167$ mg/cm^3) was prepared under the conditions of slow solvent evaporation and the fourth one was prepared by mechanoactivation.

It was shown that required curve shape can be obtained by means of silica impregnation from laevomycetin alcohol solution during sufficiently slow solvent evaporation and mechanoactivation of silica and laevomycetin as well. Herewith impregnation is more preferable due to its facility of desorption process rate controlling step.

1. S. Ummadi, B. Shravani, N.G. Raghavendra Rao, Int. J. Ph. Sci. **3** (2013) 258.
2. T.V. Krupska *et al*., Ads. Sci. Tech. **36** (2018) 300.

Study of the physical-chemical and sorption properties of SnO_2 prepared by mechanochemical and microwave routes

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There are many methods for synthesis of tin dioxide SnO_2, namely sol-gel, precipitation. However, these methods do not allow to regulate the physical-chemical properties in wide limits in the synthesis stage. The most commonly obtained samples are predominantly microporous as a rule. On the other hand, the meso-macroporous structure is required for the effective use of tin dioxide in sorption processes. The mechanochemical (MChT) and microwave (MWT) treatments can be used for eliminating mentioned above disadvantages. Therefore, the purpose of this work was to study the influence of the MChT and MWT on the physical-chemical and sorption properties of SnO_2 prepared by heterogeneous and homogeneous precipitation.

The initial and modified samples correspond to the composition $SnO(OH)_x$ (where $0.908<x<1.146$). MChT of all samples leads to partial removal of OH-groups. The initial samples are characterized by high values of specific surface area and high content of micropores. The specific surface area, total and sorption volume of pores, mesoporous size are increased as a result of MChT and MWT. Formation of the secondary porosity that presented by meso- and macropores is peculiarity of xerogel milling in water.

Sorption studies have shown that under the most optimal conditions for the sorption of U(VI) ions (pH=5-6, no background, cationic forms of uranium), the cation exchange capacity for the initial sample and the sample after the MChT were 0.82 and 2.9 mEq/g UO_2^{2+}, respectively. MChT results in significant increase the sorption capacity of U(VI) ions to the level of the standard cation-exchange resins and inorganic sorbents.

In case of sorption on the background of 0.1 M $NaHCO_3$ (pH 8, model of block water of the Chernobyl Nuclear Power Plant), the sorption capacity for both precipitated and modified samples was 0.3 mEq/g UO_2^{2+}. Under these conditions, ions of U(VI) are present in the solution as anionic carbonate complexes and the sorbents demonstrate anion-exchange properties, which are determined by number of anion-exchange centers, presumably Sn-OH groups.

Thus, MChT and MWT treatments leads to the significant improvement in the physical-chemical and sorption properties of tin dioxide, which significantly expands the scope of practical application of this versatile material.

Thermal decomposition behaviour of plastering and cement building materials modified by biocides composition for veterinary medicine

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The basis of the structural elements of modern industrial and residential buildings is concrete and cement. The physical and chemical properties of concrete depend strongly on the presence of additives which are widely used for chemical and / or physical impact on concrete mixture for the purpose of changing the properties of fresh or hardened concrete. For load-bearing structures, only chemical substances that meet the requirements of the «Temporary instructions for testing additives to concrete mixtures and subsequent registration of passports» must be used. The annex to these Guidelines contains recommendations for checking the correctness of the choice of the composition of the concrete mixture for compliance with the requirements for strength, volume stability, air pockets, shrinkage, *etc*. These tests are necessary, since additives can adversely affect concrete. Depending on the composition of the concrete, the technology of its placement and the amount of additives used, they can reduce its strength or contribute to the development of concrete tendencies for shrinkage.

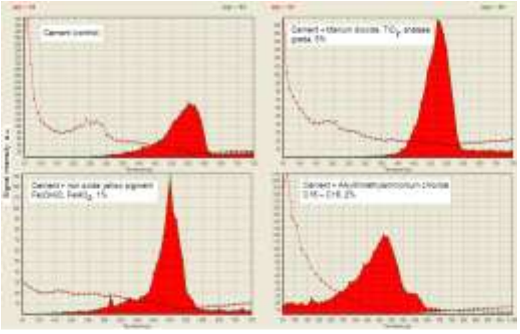

Fig. Thermograms of CO_2 ions obtained from the concrete samples modified by the different additives

It is proposed to use the TPD-MS method to predict the direction and intensity of the effect of some biocidal additives on the physico-chemical parameters of concrete used for the construction of cattle-breeding farms.

Influence of structure and properties of active carbons on dyes adsorption – equilibrium and kinetics

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Dyes are commonly used in the textile, paper, rubber, plastics, leather, cosmetic, pharmaceutical and food industries. Thus, regarding their wide usage the wastewaters containing dyes become a serious problem for the environment. Dyes are comparatively well soluble in water, poorly biodegradable, mostly toxic and carcinogenic [1]. Therefore, they should be carefully removed from water and sewage.

Adsorption methods are widely used in the processes of impurities removal from air, water and wastewaters. The use of active carbon as an adsorbent allows for efficient elimination of contaminations, especially organic ones, including dyes [2, 3]. The adsorption effectiveness depends on many factors related to the properties of adsorbent and adsorbate, the process conditions (pH), temperature, mixing rate and the presence of other substances [4, 5].

The main aim of the study was to investigate the influence of structure and properties of active carbons on the kinetics and equilibrium of adsorption of selected dyes. The series of carbonaceous materials of differentiated properties were obtained and characterized using various techniques. The adsorption isotherms and concentration profiles were measured and analyzed by applying the selected equations and models. The relationships between adsorbent and adsorbate properties, and adsorption effectiveness were analyzed.

Acknowledgements

The research leading to these results has received funding from the People Programme (Marie Curie Actions) of the European Union's Seventh Framework Programme FP7/2007-2013/ under REA grant agreement n° PIRSES-GA-2013-612484.

1. M.F.R. Pereira, S.F. Soares, J.J.M. Orfao, J.L. Figueiredo, Carbon **41** (2003) 811.
2. C. Moreno-Castilla, Carbon **42** (2004) 83.
3. D. Das, V. Gaur, N. Verma, Carbon **42** (2004) 2949.
4. G. Vijayakumar, R. Tamilarasan, M. Dharmendirakumar, J. Mater. Environ. Sci. **3** (2012) 157.
5. B.K. Suyamboo, R.S. Perumal, IJEE **3** (2012) 23.

Preparation and comparison of structural and adsorption properties of active carbons obtained from nutshells

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From several waste materials, *e.g.* agricultural wastes containing significant amounts of coal, the carbonaceous adsorbents may be obtained. They may be successfully used as adsorbers of toxic substances from air, water and sewage. These materials may reveal similar sorption properties as the carbon adsorbents obtained from traditional precursors [1-4].

The main aim of the study was preparation of a series of active carbons from nutshells as low cost adsorbents and analysis of their structural and adsorption properties. The initial material was chemically activated and carbonized. The structural properties of the obtained adsorbents were determined from nitrogen adsorption/desorption isotherms, the specific surface area, volume and size of pores were calculated. In order to determine the suitability of the obtained materials for the processes of removing impurities from water, the adsorption equilibrium isotherms and kinetic curves were measured. Studies of adsorption equilibrium were performed for 4-nitrophenol (4-NPh), 4-nitrobenzoic acid (4-NBA), 4-chlorophenoxyacetic acid (4-CPA), 2,4-dichlorophenoxyacetic acid (2,4-D), methylene blue (MB) and crystal violet (CV). Experimentally determined adsorption isotherms and concentration profiles were analyzed using simple equilibrium and kinetic equations. It was found that pyrolysis of organic wastes is easy, cheap and prominent way to obtain activated carbon. It was shown, that the way of activation and the temperature of carbonization have significant effect on the properties of carbons.

Acknowledgements
The research leading to these results has received funding from the People Programme (Marie Curie Actions) of the European Union's Seventh Framework Programme FP7/2007-2013/ under REA grant agreement n° PIRSES-GA-2013-612484

1. S.S.Z. Hindi, IJMER **2** (2012) 1386.
2. M. Singanan, Sci. Asia **37** (2011) 115.
3. T. Tay, S. Ucar, S. Karagöz, J. Hazard. Mater. **165** (2009) 481.
4. B. Sivakumar, C. Kannan, S. Karthikeyan, Rasayan J. Chem. **5** (2012) 321.

Biopolymer/porous silica support: spectroscopic characteristics of biocomposite surface

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The composites biopolymer/porous silica have many different applications, ranging from pharmaceuticals to biomaterials, biochips and biosensors. Therefore, taking into account their utility the important issue is to know/understand interactions between the surface of silica carriers and the biopolymer molecules, in order to better control the biomolecules adsorption on different surfaces of solid carriers [1].

In the study, the interactions between the albumin molecules and the surface of MCF silica particles were investigated. In order to estimate the structure of albumin/silica material, the UV-visible diffuse reflectance spectroscopy (UV-Vis DRS) was used. The obtained results provide that, the MCF surface is covered by bovine serum albumin (BSA) molecules. Upon BSA adsorption, the UV-Vis DR spectra demonstrates two absorbance bands: a narrow band with a maximum absorption located at ~229 nm and broad band with a maximum absorption situated of about ~279 nm, respectively. The maximum of the spectrum of BSA located at ~279 nm corresponds to transition of the aromatic amino acid residues: tryptophan, tyrosine and cysteine (*i.e.* disulphide bonds). Furthermore, the maximum of spectrum at ~ 229 nm is attributed to the $n \rightarrow \pi^*$ transition of the carboxylic group in peptide bond [2]. The changes in terms of the physical interactions between the protein molecules and the silica surface were verified by using ATR-FTIR infrared spectroscopy. Considering the ATR-FTIR results before/after BSA adsorption layer, it is clearly visible that the albumin molecules have been adsorbed on the surface of mesoporous carrier. It was found from the ATR-FTIR spectrum that BSA/MCF biocomposite exhibits the peak-I located at 1658 cm^{-1} for the amide-I band and the peak-II located at 1532 cm^{-1} for the amide-II band [3].

Acknowledgements

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1. J.J. Kirkland, F.A. Truszkowski, R.D. Ricker, J. Chromatogr. A, **965** (2002) 25.
2. M. Voicescu, Y.E. Khoury, D. Martel, M. Heinrich, *et al*., J. Phys. Chem. B **113** (2009) 13429.
3. W.K. Surewicz, H.H. Mantsch, Biochim. Biophys. Acta **952** (1988) 115–130.

AFM and STM investigations of nanoparticles used to improve chemotherapy effectiveness

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Application of C_{60} fullerene has been recognized as one of the most effective anticancer agents [1]. It is promising to investigate the effects of complexation between C_{60} and chemotherapeutic drug for cancer treatment Cisplatin [2] in physiological solution (PS, 0.9% NaCl) as a first step prior to further extended biological testing of the mixture of these drugs.

We report the first study of Cis molecules deposited from physiological solution. The results obtained using atomic force (AFM) and scanning tunneling microscopies (STM) provide the basis for further examination of the complexation between C_{60} fullerene and Cis in PS.

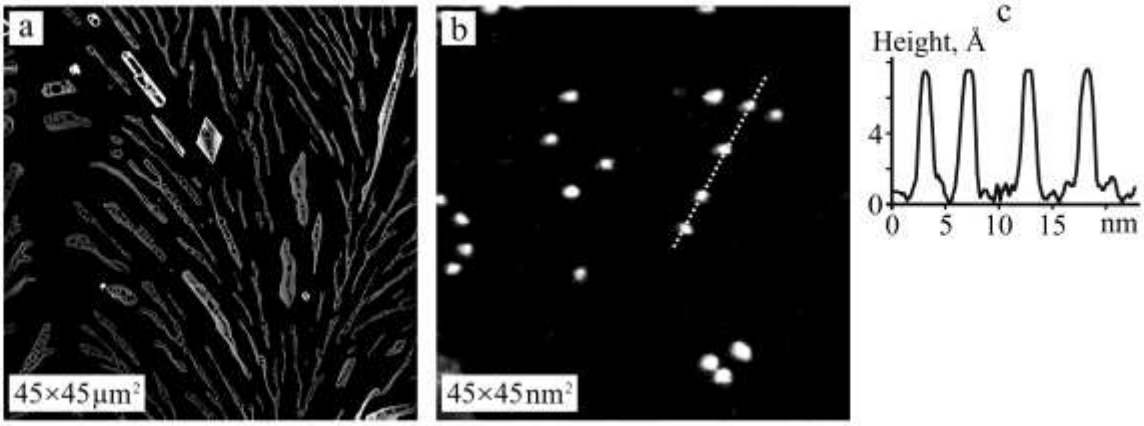

Fig. AFM image of submonolayer Cis-molecules film deposited from Cis+PS solution on mica surface (*a*); STM-image of single Cis molecules deposited from Cis+PS solution on Au (111) surface: scanning parameters: I_t=93 pA, U_t=713 mV (*b*). Cross-section along dotted line on *b* (*c*)

Acknowledgements
This work was supported by STCU project #6256.

1. S.V. Prylutska, A.P. Burlaka, Y.I. Prylutskyy, U. Ritter, P. Scharff, Exp. Oncol. **33** (2011) 162.
2. A.-M. Florea, D. Busselberg, Cancer. **3** (2011) 1351.

Functional lignin-silica hybrids for water purification: peculiarities of synthesis and application

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Currently, there is a growing interest towards more efficient use of technical lignins, aromatic biomacromolecule formed as the main by-products of pulp and paper industry. Lignin-based hybrid composites were synthesized by formation of inorganic silica network through hydrolysis of tetraethoxysilane in a presence of kraft lignin. Lignins isolated by the LignoBoost technology (LBL) and by the membrane filtration (CFB) of pulping black liquors were used. Prior to the synthesis, lignin was activated with 3-aminopropyltriethoxysilane in the presence of formaldehyde (Mannich reaction).

FTIR spectroscopy confirmed the formation of Si-O-Si polymeric network in the presence of lignin polymer. Thermogravimetric analysis demonstrated that in designed hybrids, lignin content (weight) is not higher than 79% for LBL-Si and 73.7% for CFBL-Si composite samples. That is in good agreement with results of XPS analysis, which confirmed the ratio of silicon and carbon atoms on the hybrid material's surface. Obtained hybrids belong to microporous materials with some amount of mesopores in their structures, which is in a good agreement with IUPAC recommendations for sorbents. Cumulative volume of pores in hybrid composites has increased in several times (for LBL-Silica in 4 times, CFBL-Silica in 37 times) in comparison with initial lignins and pure silica.

The adsorption capacity of hybrid composites towards Methylene Blue dye is higher than that for the initial lignins. In case of LBL such increase reached 30% (adsorption capacity of LBL-silica = 41.6 mg/g) and in the case of CFBL lignin the adsorption capacity was almost doubled (adsorption capacity = 58.9 mg/g). Such improvement in the sorption capacity of hybrid materials is due to the immobilized lignin.

Acknowledgements

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MALDI and GALDI mass spectrometry investigation of fragmentation of zirconium and hafnium phthalocyanines with out-of-plane ligands

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The interest in the synthesis and research of phthalocyanine complexes has increased in recent years due to their application in medicine, microelectronics, sensors, photonics, *etc*. We developed methods for the modification of phthalocyanine complexes of zirconium and hafnium by ligand exchange reactions at the central metal atom of the macrocycle made it possible to obtain a significant number of complexes with out-of-plane ligands: various β-dicarbonyl compounds, including such sterically hindered ones as methoxydipivaloyl methane, isopropylacetoacetate, pyrazolone derivatives; catecholates; carboxylates.

The main problem of analyzing these compounds is their low solubility in organic solvents; it complicates the determination of their exact composition and structure. Therefore, the mass spectrometry of such compounds can be useful for their investigation. We succeeded in fixing the molecular ions of some out-of-plane coordinated phthalocyanine complexes of zirconium and hafnium by MALDI and GALDI mass spectrometry.

The most informative were studies of β-dicarbonyl complexes of phthalocyanines of zirconium and hafnium. Molecular ions peaks $[PcML_2]^+$, as well as ions $[PcML]^+$ and $[PcM{=}O]^+$, are observed in their mass spectra. In the case of out-of-plane coordinated catecholate ligands, molecular ions $[PcML]^+$ and peaks corresponding to $[PcM{=}O]^+$ are also observed. For *bis*-carboxylate complexes of phthalocyanines, the molecular ions $[PcML_2]^+$, as well as the fragmentation products $[PcML]^+$ and $[PcM{=}O]^+$, were not detected using different regimens of registration. Thus, the use of MALDI and GALDI mass spectrometry is applicable for the analysis of only some out-of-plane coordinated complexes of zirconium and hafnium phthalocyanines.

Fluctuations of different nature in the theory of high-temperature ratchets

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It is well known that external perturbations of different nature can entail fluctuations of potential energy of Brownian particles and, hence, transform them into Brownian ratchets. We investigate the influence of fluctuations types on ratchets' characteristics. The fruitful analysis became possible due to analytical solution of the Smoluchowski equation obtained in the form of a power series in the inverse friction coefficient [1], that gave the series form for the main ratchet characteristics, its average velocity. We show that for a driving force $F(x,t) = -\partial U(x,t)/\partial x$ ($U(x,t)$ is a particle potential energy) of a general additive-multiplicative form $F(x,t) = \sum_{r=1}^{N} \sigma^{(r)}(t) f^{(r)}(x)$, the velocity is determined by correlation functions of different orders, through the integrals $\int_0^\infty d\tau_1 \int_0^\infty d\tau_2 \ldots$ $\int_0^\infty d\tau_n \left\langle \sigma^{(r_1)}(t)\sigma^{(r_2)}(t-\tau_1)\ldots\sigma^{(r_n)}(t-\tau_1-\ldots-\tau_{n-1})\sigma^{(r_{n+1})}(t-\tau_1-\ldots-\tau_{n-1}-\tau_n)\right\rangle$, and the nature of the time-dependent quantities $\sigma^{(r)}(t)$ differs the operation of averaging over the fluctuations, $\langle \ldots \rangle$. The correlation functions of the low order determine the velocity of high-temperature ratchets, and the summation is confined to $n = 1, 2$ for pulsating ratchets. For them, with $U(x,t) = u(x) + \sigma(t) w(x)$, we analytically analyze the following processes $\sigma(t)$: deterministic periodic ($\sigma(t) = \sigma(t+\tau)$), stochastic *N*-state Markovian (with time-independent rate constants $\gamma_{nn'(n'n)}$ of transitions $\sigma_n \rightleftarrows \sigma_{n'}$ between values σ_n, $n = 1, 2, \ldots, N$, of stochastic variable $\sigma(t)$), stochastic Markovian and non-Markovian dichotomous noises ($N = 2$). The results are used for the detailed analysis of real ratchet systems with a spatial harmonic signal as a fluctuating (governing) part of the potential: planar dipole rotor in a two-well symmetric potential of the hindered rotation; saw-tooth stationary potential, perturbed by a spatial harmonic signal; deterministic processes of a relaxation type. The comparison of the influence of Markovian and non-Markovian dichotomous fluctuations on ratchet behavior is presented.

1. V.M. Rozenbaum, JETP Lett. **88** (2008) 342.

Hidden symmetries of pulsating ratchets

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In the theory of Brownian ratchets a question of a principle importance is that of their symmetry properties. The absence of directed motion under the broken both thermal equilibrium and reflection symmetry is a fact to consider the ratchets more closely, as the suppression of the ratchet effect can be the display of hidden symmetries in the system. The classical symmetry analysis, based on the analysis of Langevin-type equations, cannot reveal hidden symmetries, so one has to analyse the solutions of the equations (Smoluchowski, Langevin). Getting these solutions requires cumbersome mathematics as a rule. We analyse hidden symmetries of pulsating ratchets using an iterative representation (analytical) of the ratchet average velocity in the form of a power series

$$v\left\{F(x,t)\right\}=\sum_{n=1}^{\infty} i^n \zeta^{-n-1} \sum_{q_1 j_1 \dots q_n j_n} \frac{k_{q_1}\dots k_{q_1+\dots+q_n} F_{q_1 j_1}\dots F_{q_n j_n} F_{-q_1-\dots-q_n,-j_1-\dots-j_n}}{\left(i\omega_{j_1}+Dk_{q_1}^2\right)\dots\left(i\omega_{j_1+\dots+j_n}+Dk_{q_1+\dots+q_n}^2\right)},$$

F_{qj} are the Fourier components of an applied force $F(x,t)$, D and ζ are the diffusion and friction coefficients, $k_q=(2\pi/L)q$, $\omega_j=(2\pi/\tau)j$. We discuss various symmetries of pulsating ratchets with the multiplicative applied force, $F(x,t)=g(x)\sigma(t)$, and manifestations of these symmetries in ratchets' behavior. The interplay of symmetry properties of periodic multipliers, $g(x)=g(x+L)$ and $\sigma(t)=\sigma(t+\tau)$, is analyzed; they can be symmetric, antisymmetric, and shift-symmetric functions, that is, by $\sigma(t)$, $\sigma_s(t-t_s)=\sigma_s(-t-t_s)$, $\sigma_a(t-t_a)=-\sigma_a(-t-t_a)$, $\sigma_{sh}(t+\tau/2)=-\sigma_{sh}(t)$. Two new symmetry properties of pulsating ratchets have been revealed [1]: the absence of the ratchet effect if (i) $\sigma(t)$ is *a*-symmetric, while the coordinate dependence $g(x)$ is arbitrary, and (ii) $\sigma(t)$ is *sh*-symmetric and $g(x)$ is *s*- or *a*-symmetric. As an example, in (i) one has

$$v\left\{F(x,t)\right\}=v\left\{F(x,t-t_a)\right\}=v\left\{-F(x,-t-t_a)\right\}=v\left\{-F(x,-t)\right\}=v\left\{-F(-x,t)\right\}=-v\left\{F(x,t)\right\}.$$

The two new symmetries degenerate into one non-trivial property if $\sigma(t)$ is *u*-symmetric (belongs to both *a*- and *sh*-types): if time dependence possesses *u*-symmetry, the average velocity is zero in the absence of inertia, but it can be different from zero when inertia is taken into account provided that the coordinate dependence of the potential is not *s*- or *a*-symmetric.

1. V.M. Rozenbaum, I.V. Shapochkina, Y. Teranishi, L.I. Trakhtenberg, JETP Lett. **107** (2018, to be published).

Physical processes and crisis modes when boiling water on porous metal surfaces

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A series of research results of the influence of characteristics of metal fiber coatings-capillary structures on the value of limit heat fluxes during boiling water in conditions typical for the operation of low-temperature range heat-pipes are presented. The obtained results are summarized by an empirical formula suitable for the corresponding engineering calculations.

Two-phase heat transfer devices (THD): heat pipes (HP) and their variants - thermosyphons (TS) are promising elements for efficient systems of cooling and thermostabilization of heat-stressed units of chemical equipment. When working with HP in conditions of significant density of heat fluxes $\boldsymbol{q}$ [W/m^2], the possible fact is the emergence of limit (critical) modes of heat transfer [1], which can lead to failure of the cooling system. As a result of the research, the authors received experimental data that illustrated the influence of a number of physical characteristics and parameters of copper fibrous structures (MVS) on the limit values of the densities of heat fluxes in boiling water in conditions close to the functioning of the TT and TS.

The results of research of the influence of physical characteristics and parameters of the CFS on the processes typical for the heating zones of the heat-stressed areas of chemical equipment are summarized in the form of an empirical formula that takes into account almost all the main factors influencing the critical values of the densities of heat fluxes (q, W/m^2), brought to the zones of heating HP and TS, with the operation of cooling systems created on THD basis. The resulting calculated empirical formula has the following form:

$$Q_{\mathrm{cr1}} = C \cdot q_{\mathrm{cr}} \cdot \delta^{\mathrm{n}} \cdot \lambda^{0,1} \cdot \Theta^{0,12} \cdot D^{0,2},$$

where: C=105, n=0.25 for the thicknesses of the CFS δ=0.1-0.6 mm; C=0.28, n=$-$0.55 for δ=0.6-3 mm; λ $-$ thermal conductivity of CFS; Θ $-$ porosity of CFS (from 0.4 to 0.9); D $-$ average pore size of CFS; q_{cr} (W/m^2) – critical value of density q when boiling water on smooth technical surfaces.

1. A.A. Shapoval, V.K. Zaripov, M.G. Semena. Teploenergetika, **12** (1983) 63.

Components of the energy spectrum of the interaction of a polymer-nanodispersed metal

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The nanodisperse metal filler is considered as a set of two subsystems: an ionized atom group, which forms a crystalline lattice, and an electron gas that is responsible for its electromagnetic properties. In the proposed model, we assume that the energy of a single ion-dipole interaction for a dipole of a polymer matrix when it is oriented to a metal filler surface is not significantly different for different types of metal. This is confirmed by calculations of the energy of a single connection due to the ion-dipole interaction of Fe, Ti, Cu, PS, and PVC. The data analysis showed that the maximum energy of a single-line connection in the transition from one nanodisperse metal to another in a particular polymer matrix differs by (0.5÷9.0)%.

For the composite obtained on the basis of nanodispersed metal - flexible-film polymer (PVC, PVB, PS, PMMA) the results of calculation of the unit interaction of averaged dipole with the ion of the filler are given and analyzed; the value of the specific density of ions on the polycrystalline surface of the metal; dispersion forces; the conditions for the occurrence of chemical interaction on the boundary between the phase separation of polymer and metal have been established; the possibility of formation of new functional groups, the restoration of oxides.

The value of the bond strength at the boundary of the phase separation is calculated for a polymer - a nanosized metal, taking into account the atomic volume of the metal, the radii of their atomic nuclei. It is shown that the nature of the interaction of a polymer with a nanodispersed metal filler is essential for directional control of the complex of properties of a composite due to the manifestation of its action by the induction mechanism. The hypothesis that the decrease in the mobility of the atoms of the matrix due to their interaction with the active centers of the filler surface causes the polarization of the C-Cl- (PVC) bond, is the first stage in the reaction of its dechlorination. The concentration dependence of the activation energy of the polymer thermal degradation process on the type and content of the nano-dispersed metal has the form similar to that of other investigated structural-sensitive properties (viscoelastic, dielectric, thermophysical).

Magnetic and mechanical properties of epoxy magnetocomposites

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Magnetocomposites based on epoxy resin Epoxy 520, filled with microspheres of crystalline silicon dioxide, containing up to 2.5% of the impurity of atomic iron were studied. The concentration of particles in the composites was 1.5%, the average size was 10-20 µm, the specific surface area was 2.2-3.2 m^2/g. The microspheres were coated with a conductive polymer – polyaniline with a conductivity of 1.8×10^{-2} $\Omega^{-1}cm^{-1}$ and a dielectric polymer – polyvinylchloride with a conductivity of no more than 10^{14} $\Omega^{-1}cm^{-1}$.

The measurements of the magnetic saturation moment M_s and the coercive force H_c were performed by magnetic granulometry. They showed that in the particles the iron atoms are in the magnetic ordering (probably antiferromagnetic) state with the parameters M_s = 6.5 emu/g and H_c = 33 Oe. The particle encapsulation in the conducting and dielectric polymers reduces the parameter M_s to values 3.2 and 5.7 emu/g and increases the H_c to 49 and 42 Oe, respectively.

The study of magnetic composites under pressure showed that their load curves have three range: elastic pressure, conformational deformation and viscoelastic deformation with fracture. The behavior of the elastic loading parameters, namely loading (σ), the Young's modulus (E) and the thermal stability of the composites is correlated. For the initial composite $\sigma = 1238$ kgf/cm^2, $E = 1.5\cdot10^4$ kgf/cm^2, while for the composites with polyaniline–coated microspheres, the σ and E magnitudes grow respectively in 1.13 and 1.06 times, and for the particles coated with polyvinylchloride both parameters decrease in 0.95 times.

Resume. Encapsulation of particles leads to a decrease in the penetration of the magnetic field into a particle and reduction of M_s and the appearance of magnetic centers with unpaired spins on the interphase surface. The interaction of centers with iron atoms leads to pinning domain walls and increasing of H_c. Sites, possibly, have different a charge, since encapsulation in polyaniline enhances the strength of the composite structure, and the coating with polyvinylchloride weakens the structure strength.

Electrophysical properties of composites based on the epoxy resin and thermally expended graphite

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To date, a variety of different types of composite materials have been obtained on the basis of polymers. It has been introduced in various industries for the manufacture of various types of protective coatings, refractory materials, electronic and optical devices, which, however, do not fully meet the ever-increasing requirements, namely: moisture resistance, incombustibility, durability, technology, conformity to weight criteria, affordability by the price.

The purpose of this work is to determine the optimal concentration of thermo-expanded graphite (TEG) for two composites: perlite - epoxy resin and vermiculite - epoxy resin.

Two series of specimens were made: one having a low content of vermiculite, the other one – the same of perlite; in both series, the content of the filler - TEG (from 0.1 to 2% by weight) was variable, the epoxy resin was used as the binding agent. Electrophysical characteristics - dielectric permittivity ε' and specific electrical conductivity σ were measured at low frequencies of 0.1, 1 and 10 kHz by two-contact method with the help of the immittance meter E7-14. Some measurement results are given in Table, ε'_{10} is determined at a frequency of 10 kHz, and σ_1 is determined at a frequency of 1 kHz. Relative error did not exceed ±5%.

Table. Electrophysical characteristics of composites with TEG

TEG content, %	Perlite-based Composites		Vermiculite-based Composites	
	ε'_{10}	σ_1, Ohm^{-1}cm^{-1}	ε'_{10}	σ_1, Ohm^{-1}cm^{-1}
0.1	12.5	$4.7\cdot10^{-10}$	16	$4.4\cdot10^{-10}$
0.57	57.5	$6.9\cdot10^{-7}$	123	$3.5\cdot10^{-4}$
1	316	$2.65\cdot10^{-5}$	1180	$2.6\cdot10^{-3}$
1.5	3087	$7.5\cdot10^{-3}$	4420	$7.2\cdot10^{-2}$

The percolation threshold determined from the percolation equation is of 0.35% (0.0018 of volumetric content of the TEG) for the vermiculite system and 0.75% (0.0039) for the perlite system.

Thus, the difference in electrophysical characteristics of the two systems for the same TEG content is due to the nature of the surface of the dielectric constituents. Changing the content of such dielectric ingredients allows us to expand the functionality of composites used for shielding from electromagnetic fields.

Supramolecular sorbents based on silica gels and crystalline cellulose modified with polyhexamethyleneguanidines

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The development of new surface-modified materials by grafting of certain functional groups to the carrier surface contributes to solving many problems of science, engineering and technology. The preparation of such materials in many cases is associated with the complexity of implementing modification processes, need to conduct them in non-aqueous solutions, high cost of modifiers, *etc*., which limits their practical application.

We have shown that to overcome these obstacles, it is possible to use the modification of dispersed oxides, in particular silica gels, and crystalline cellulose (CC) with polyhexamethyleneguanidine (PHMG). The commercial product polyhexamethyleneguanidine hydrochloride (PHMGH) is characterized by a set of polymer chains, mainly with n = 30-90. The formation of PHMGH adsorbates is carried out through interaction of highly basic amino groups of PHMGH (pK_a = 13.5), which are protonated in wide range pH and capable of forming hydrogen bonds with the hydroxylated surface. Quantitative extraction of PHMGH by silica gels occurs in a pH range from 2 to 8 while by CC – only in a pH range 6-9. This difference in PHMGC sorption behaviour can be explained by different bond strengths, since the pK_a of silica gel hydroxyl groups is 7.1, and CC is 10, 12 – for the secondary groups and 14 – for the primary groups.

Using the capillary electrophoresis method it has been shown that low molecular weight PHMGH oligomers are completely desorbed by hydrochloric acid solutions, while PHMGH oligomers with longer chains do not desorb even with concentrated hydrochloric acid solutions. Sorption of PHMGH on cellulose, unlike silica, is completely reversible.

The supramolecular structures formed on the surface are capable of attaching anionic compounds, such as sulfonated dyes, with the formation of supramolecular structures: $Sorbent\cdots PHMGH\cdots SO_3R^-$ which in turn are capable of coordinating metal ions or other cationic compounds. All bonds between the components of supramolecular structures are non-covalent. By regulating hydroxyl groups pK_a, adsorbate constituents sorption/desorption conditions, it is possible to solve a number of analytical problems using hybrid or combined analysis methods.

Influence of bentonite nanoparticles and nano-SiO_2 on the total content of the phenolic compounds in the cultural medium of bacteria *Azotobacter vinelandii* IMV B-7076

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Among natural nanomaterials – bentonite is found quite often in sediments and soils [1]. This clay mineral can affect on promising strains of microorganisms at introducing them into the agroecosystem. Nano-SiO_2 can induce an increase in the level of reactive oxygen species in living systems [2].

It was interesting to investigate the effect of bentonite nanoparticles and nano-SiO_2 on the total content of phenolic compounds (Ph-OH) in the culture medium (CM) of *A. vinelandii* IMV B-7076 that is a highly effective component of the complex bacterial preparation Azogran. Since phenolic compounds are an integral part of the antioxidant system of any living organism.

It was established that at cultivation of the strain *A. vinelandii* IMV B-7076 with 0.05 – 0.5 g/L of bentonite nanoparticles, the content of Ph-OH in its CM exceeded the total amount of phenolic components in CM of control on 32.1 – 16.5%. However, when growing of study bacteria with silica nanoparticles an increase in the number of phenols in the CM of *A. vinelandii* IMV B-7076 was observed only in variants with 0.05 – 0.1 g/L of nano-SiO_2. At introducing into a nutrient medium 0.5 g/L of silica nanoparticles the quantitative index of Ph-OH in the CM of *A. vinelandii* IMV B-7076 decreased, compared with the control variant, by 3.8% (Table).

Table. Influence of bentonite nanoparticles and nano-SiO_2 on the total content of phenolic compounds in culture medium of *Azotobacter vinelandii* IMV B-7076

Content of nanoparticles, g/L	Total content of phenolic compounds, μg/mL			
0	Bentonite	85.1 ± 3.2	nano-SiO_2	52.3 ± 2.7
0.05		117.2 ± 4.5		61.8 ± 5.7
0.1		112.5 ± 2.8		57.6 ± 2.8
0.5		101.6 ± 4.8		48.5 ± 9.5

1. K. Emmerich, F. Walters, G. Kahr, G. Lagaly, Clay Miner. **57** (2009) 101.
2. Yu Shang, Tong Zhu, Yi Li, JinCai Zhao, Science in China Series B: Chemistry. **52** (2009) 1033.

Study of ornidazole desorption from the nanocomposites based on silica

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The problem of effective complex therapy of infectious diseases is among the most pressing challenges in modern medicine. Currently, antibiotics belonging to the 5-nitroimidazole group, in particular ornidazole, are among the most effective medicines due to the fast bactericidal effect, low inhibitory concentration in relation to bacteria, and low toxicity.

The kinetics of ornidazole release from composite materials was studied in this work. The composites were obtained by impregnation of pyrogenic silica with a specific surface of 300 m^2/g with ornidazole from the aqueous and alcohol solutions thereof. The content of antimicrobial agent was 2, 4 and 12 % by weight.

The release of the active substance was carried out in accordance to the standards of the Pharmacopeia of Ukraine on a device with a basket for dissolving solid dosage forms into distilled water with volume of 1000 ml at the temperature of 37 °C. Quantitative determination of ornidazole was carried out by a spectral method at a wavelength of 314 nm.

The analysis of ornidazole release profiles for the studied composites showed a similar nature of the kinetic curves for all composites. The release of ornidazole was more than 80 % after 15 minutes of dissolution test.

Effect of doping with zirconium incorporation on the properties of defect titanium dioxide films: quantum chemical calculations

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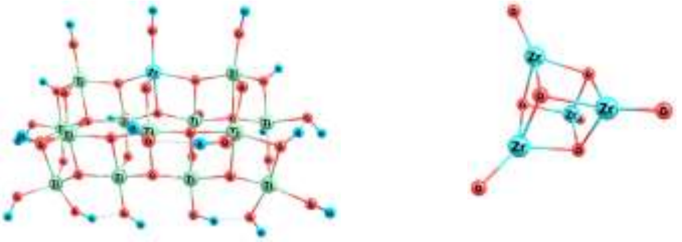
One of the promising materials for photocatalysis is titanium dioxide TiO_2. Such a great interest to this substance is mostly due its physical and chemical properties.



Molecular models for defect titania ($Ti_{13}ZrH_{22}O_{39}$) and for zirconia (Zr_4O_8)

Zirconium is known to be a chemical analog of titanium and almost always is present as an impurity in its natural compounds and significantly affects their properties. Removal of zirconium from titanium dioxide related materials is often a complicated technological problem. It is possible to detect the presence of a zirconium impurity in titania using spectral methods (vibrational and electronic spectroscopy). A correlation between the defect structure, features of its nearest coordination environment, and experimental spectra can be established by theoretical modeling using quantum chemical methods.

In this work, the vibrational and photoelectron absorption spectra of titanium dioxide structures (pure and containing zirconium dioxide) and pure zirconium dioxide have been calculated (DFT/B3LYP/3-21G**). In the calculations, a cluster approximation was used using molecular models with the composition of $Ti_{13}ZrH_{22}O_{39}$ and Zr_4O_8. As a result of calculations, it has been found that for the Zr_4O_8 cluster, the vibrations in the region of 583.6 cm^{-1} correspond to the "breathing" vibrations of Zr-O bonds. Consequently, for the cluster of $Ti_{13}ZrH_{22}O_{39}$, the bands within 527-539 cm^{-1} can be attributed to the vibrations of the zirconium atom. As can be seen from the calculations of the Zr_4O_8 cluster, in the photoelectron spectrum, the peak in the 321.9 eV region correspond to the Zr3*p* energy level whereas for the $Ti_{13}ZrH_{22}O_{39}$ cluster the corresponding band is slightly shifted (up to 321.8 eV).

Thus, we can conclude as follows: in the photoelectron spectrum, the absorption band Zr3*p* is characteristic and weakly depends on the chemical environment of the zirconium atom.

Photo- and electrocatalytic activity of TiO_2 based films: effect of metal ion's doping

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Nanostructured TiO_2 films doped with metal ions (Zn, Zr, Co, Ni, Mn, Cu or Fe) were synthesized by sol-gel method. The films were characterized by hexane adsorption, XRD, XPS, Raman and UV-Vis spectroscopy. Band gap energy and the position of flatband potentials were estimated by photoelectrochemical measurements. Herein, we analyzed the effect of metal ions' doping of TiO_2 films on their structural and optical properties as well as electro- and photocatalytic activity.

Doping with metal ions has been employed to tune the electronic structure and enhance the photocatalytic activity of titania based materials under both UV and visible light. Increasing 3*d* metal ions content in TiO_2, the optical band edge shifts to lower energy. The largest shift was observed for Fe-doped TiO_2 film. In turn, the characteristic bands registered in diffusion reflectance spectra indicated the formation of Co_3O_4 spinel phase; $NiTiO_3$ and Mn_2O_3 phases after calcination at 650 °C. XRD patterns showed the anatase nanocrystalline (8–20 nm) phase for the films calcined at 450 C. The higher degree of anatase-to-rutile transformation was observed for Mn and Cu doped titania films compared to Co, Ni and Fe ones. As shown by XPS spectra, the Ti–O–M bonds were formed for all samples. The higher adsorption ability of the films was proposed to be connected with the formation of these common bonds.

Energy level diagrams of synthesized films were designed by the direct electrochemical measurements that allowed predicting the activity of the semiconductors in the photocatalytic and electrocatalytic processes. The films containing 1% of Zn, Zr, Co, Ni, Mn or Cu ions showed much higher photocurrent quantum yield than that for pure titania. The enhancement in photocurrent efficiency of metal doped electrodes indicates that M^{n+} ions addition is beneficial to promote the charge separation within mesoporous TiO_2 film. The lower photocurrent quantum yield was noticed for the iron doped films with the maximum photocurrent response in the visible range. The presence of metal ion's were responsible for the cathodic shift of the bottom of conduction band along with E_g decrease leading to the high efficiency in photocatalytic process and electrocatalytic reduction of dissolved oxygen.

Adsorption removal of dyes from aqueous solutions using low cost adsorbents based on agro-industrial waste products

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Wastewater of textile, printing, leather, cosmetic and others industries contains synthetic dyes and they pose a serious threat to human health. This is due to the fact that dyes can cause allergic dermatitis, skin irritation, mutation, cancer, *etc*. Nowadays there are various techniques for the removal of dyes from wastewater. However, the high effectiveness of adsorption for dye removal from wastewater has made it an alternative to other treatment methods.

Widespread introduction of the adsorption in treatment of the wastewater containing of dyes is impossible without new effective adsorbents which should be cheap and affordable, as well as environmentally friendly. Besides, in many countries one of the most important problems is the sensible use of agro-industrial waste, because most of them are unclaimed and burned. The problem can be solved if it would be obtained new inexpensive adsorbents based of annually reproducible and environmentally safe agro-industrial waste products as alternatives to expensive activated carbon.

The main goal of this paper is to provide a summary of recent investigations carried out by numerous researchers (from 2008 to 2017) concerning the use of agro-industrial waste products for the removal of synthetic (cationic and anionic) dyes from wastewater of different industries.

An extensive list of adsorbents prepared from different types of raw, activated and modified agro-industrial waste has been compiled and full study of comparison adsorbent properties has been carried out. Advantages and disadvantages of the adsorbents, optimal conditions of adsorption, and adsorption capacities of the adsorbents are presented.

Thus, the analyses of the investigations indicated that adsorbents based on agro-industrial waste can be used in the wastewater treatment process and the removal efficiency of dyes may be as high as 100%. However, the process of adsorption requires further investigation in the direction of modification of the agro-industrial waste for enhanced their adsorption capacity, modelling of adsorption process, regeneration and recycling of adsorbents. On the other hand, in further more interest should be concentrated by the researchers to predict the performance of the adsorption process for dye removal from real industrial effluents.

The peculiarities of CuI formation on the surface of ZnAl layered double hydroxides

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Cuprous iodide (CuI) has attracted much attention in the past few decades owing to its unusual characters such as large direct band gap (3.1 eV below 350°C), negative spin-orbit splitting, unusually large temperature dependency, anomalous diamagnetism behavior, large ionicity, new high pressure phase and potential applications in superionic conductors, solid-state solar cells, catalysis for synthesis of organic compounds. Layered double hydroxides (LDHs), also known as hydrotalcite-like compounds or anionic clays, form a large class of layered materials. The layered structure and the anion-exchange properties of LDHs make them attractive as hosts because of their potential applications in areas such as catalysis, separation, sensors, electrochemistry, and bionanotechnology. CuI supported on ZnAl LDHs were synthesized by interaction of iodide intercalated ZnAl LDHs with aqueous solution of Cu^{2+} ions. The formation of CuI on the surface of LDHs depends on the molar ratio of LDHs:I^-. γ-CuI was formed on the surface of ZnAl LDHs at LDHs: I^-=1:2 for LDHs with Zn:Al ratio 2:1, 3:1 and 4:1 (Fig. *a*). The intercalation of triiodide/iodide redox couple was observed for Zn_2Al LDHs at lower LDHs: I^- ratios (Fig. *b*).

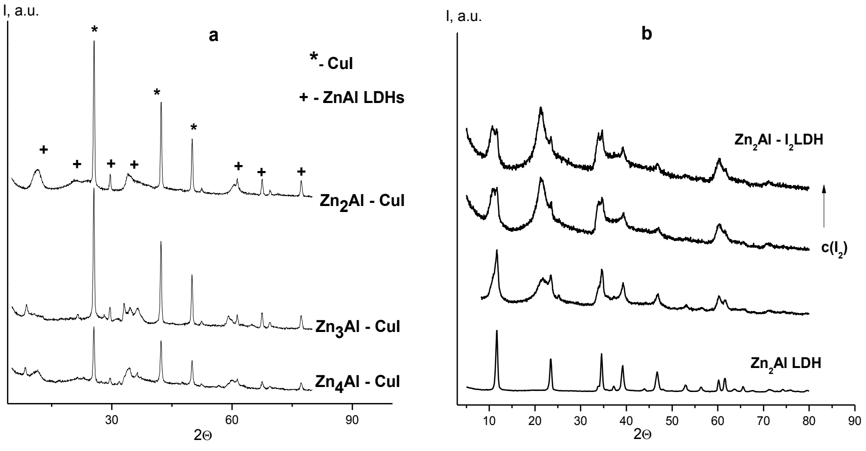

Fig. XRD patterns of ZnAl LDHs

The intercalation of the triiodide/iodide redox couple on micrometric LDHs can be used for the substitution of liquid electrolytes with organic hole transporting materials and solvent-free polymer electrolytes [1].

1. M. Bastianini, D. Costenaro, C. Bisio, L. Marchese, U. Costantino, R. Vivani, M. Nocchetti, Inorg. Chem. **51** (2012) 2560

Magnetic fluid with high dispersion for hyperthermia purpose

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One of the more promising biomedical applications of magnetic nanoparticles is cancer therapy via magnetic hyperthermia. Cancerous tissue has been shown to have a higher sensitivity to heat due to decreased blood flow and therefore higher acidity, thus allowing most cancerous cells to be destroyed in the 42–45°C range while healthy cells remain relatively unchanged [1].

For this purpose we synthesized stable magnetic fluid based on Fe_3O_4 and PEG (MF, MF-PEG) with size of approximately 20 to 22 nm, a saturation magnetization of approximately 0.1 emu/g. Result of magnetic measurements, in conjunction with the high magnitude of saturation magnetization indicates that the particles are superparamagnetic.

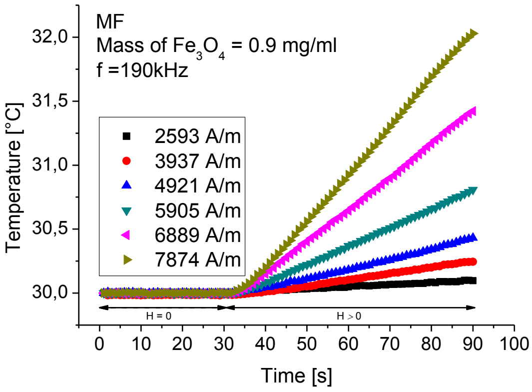

Fig. Time evolution of temperature of MF during the exposition to various AC magnetic field intensities *H* at the frequency *f* = 190 kHz

The thermal response of iron oxide nanoparticles in an alternating magnetic field was studied using calorimetric measurements. It was shown (Fig.) that the thermal output increased with higher magnetic field intensities, with a nearly linear temperature rise over a period of 60 sec. As field strength was increased from 2.6 to 7.9 kA/m, the SAR for heating fluid Fe_3O_4 particles at 190 kHz increased too (from 5.2 to 122.6 W/g).

Acknowledgements
This work was done with the support of the National Slovak Scholarship Programme for the Support of Mobility (SAIA).

1. Nguyen TK Thanh (Ed), Clinical Applications of Magnetic Nanoparticles, Taylor&Fransic: London, 2018, p. 490.

Synergism and antagonism of the action of non-ionic and cationic surfactants during their mutual adsorption on paraffin

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The actual trend of modern colloid chemistry is the study of the properties of surfactant mixtures. Of particular practical importance are the studies of the adsorption of surfactant mixtures on a solid surface, at the same time this problem is quite new and the regularities of the effect of the composition of mixtures on their adsorption from solutions have not yet been established.

The purpose of this work was to evaluate the mutual influence of non-ionic (Twins: Tween-20, Tween-40, Tween-60, Tween-80) and cationic surfactant (dodecylpyridinium chloride) upon their joint adsorption from aqueous solutions on the low-energy paraffin surface. The mole fraction (*n*) of Twins (Tw) in the solution was 0.2, 0.5; 0.8. As adsorbent, 1% paraffin suspension was used.

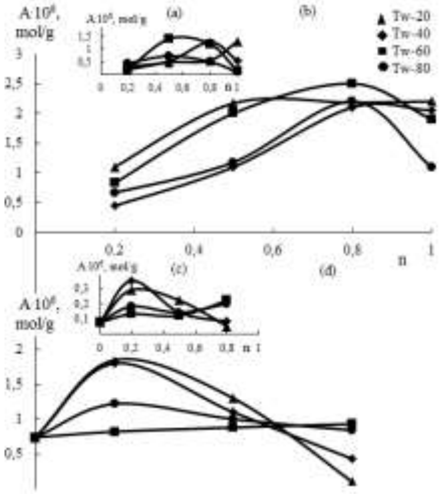

Fig. Dependence of the adsorption of Twins (*a*, *b*) and dodecylpyridinium chloride (*c*, *d*) from mixed solutions on the paraffin surface on the composition of the mixture (*a*, *b* – C_p=0.05·10^{-5} mol/dm^3; *b*, *d* – C_p=0.15·10^{-5} mol/dm^3)

In the systems under consideration, both synergistic and antagonistic effects are manifested from the adsorption of non-ionic and cationic surfactants from binary solutions, which is related to the assumed competitive mechanism of adsorption on the solid surface of paraffin. A negative effect on the adsorption of Twins with a smaller hydrocarbon radical in the molecule (Tween-20 and Tween-40) on the paraffin surface is the addition of dodecylpyridinium chloride to the solution, and for Tween-60 and Tween-80, it is positive.

A positive effect of non-ionic surfactants on the adsorption of dodecylpyridinium chloride on the paraffin surface was also established, which is manifested in an increase in the adsorption values of cationic surfactant from the mixture with Twins as compared to its adsorption from the individual solution.

Magnetite-silica materials with modified surface, synthesis and sorption abilities of organic compounds

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Magnetite-containing and silica-coated nanomaterials are very interesting subject, not only in the aspect of investigation of magnetic field influence on phenomena taking place on liquid-solid interfaces, what was previously presented by our team. Thanks to its specific physical properties, materials with enhanced magnetic susceptibility can be also used in applications where rapid separation of solid and liquid phases is needed (for example, sample preparation [1], or catalysis [2]). Adding additional magnetic force on particles signifially shortens time of solid phase particle sedimentation. The materials can be also applied when a substance must be delivered in one exact place in living organism (*e.g*. targeted drug release, gene therapy [3]).

By modifying the surface of the materials using various organic groups such as octadecyl-, vinyl-, phenyl- or aminopropyl- silyl groups their sorption properties, bioavailability and other derivative properties can be greatly expanded. It opens the possibilities to use such materials in many new applications connected with medicine, environmental protection, and many others.

In our experiments, the procedure of magnetite/silica base material synthesis was optimized, various methodologies of silica surface modifications were tested and finally, their sorption ability of representatives of various organic substances (drugs, pesticides, phenols) was tested.

1. A.A. Issa, K.A. Al-Saad, A.S. Luyt, J. Am. Ceram. Soc. **101** (2018) 2038.
2. M. Karimi, L. Ghandi, D. Saberi, A. Heydari, New J. Chem. **42** (2018) 3900.
3. A.N. Nacev, Magnetic drug targeting: Developing the Basics, Faculty of the Graduate School, University of Maryland, College Park, 2013, p. 200.

Spectroscopic and optical properties of erbium and ytterbium doped transparent silica glasses prepared by sol –gel process

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In the present work, pure transparent quartz glasses doped with erbium and ytterbium oxides (0.05 and 2 wt. %) were successfully prepared by a modified sol-gel technique. Monolithic gels are produced on the basis of synthetic SiO_2 nanoparticles with defined amount of Er_2O_3, Yb_2O_3, $Si(OC_2H_5)_4$, and gelation catalyst HCl.

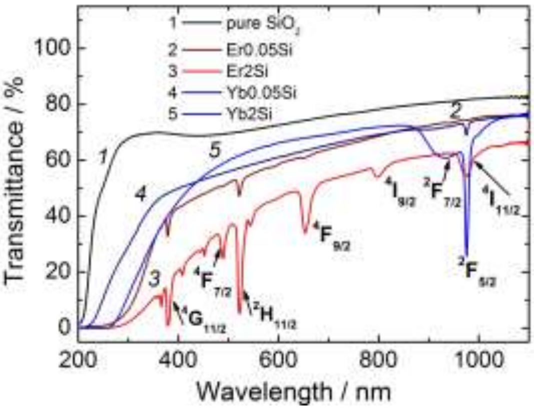

Fig. UV-vis spectra of pure (*1*) and doped sol-gel silica glasses with Er^{3+} (*2*, *3*) and Yb^{3+} (*4*, *5*)

The Raman spectroscopy was used for identification of the structural changes due to doping. The UV–Vis absorption and photoluminescence spectroscopy were applied for spectral characterization of samples. The characteristic absorption bands of Er^{3+} ions which are observed at 358, 366, 379, 408, 444, 452, 489, 521, 546, 652, 799 and 980 nm are assigned to $^4I_{15/2} \rightarrow$ $^2G_{7/2}$, $^4G_{9/2}$, $^4G_{11/2}$, $^4F_{9/2}$, $^4F_{3/2}$, $^4F_{5/2}$, $^4F_{7/2}$, $^2H_{11/2}$, $^4S_{3/2}$, $^4F_{9/2}$, $^4I_{9/2}$ and $^4I_{11/2}$ transitions, respectively (Fig. *curves 2, 3*).

The absorption peaks of Yb^{3+} are located at 930 and 976 nm respectively, which are attributed to the transitions between different Stark levels of Yb^{3+}:$^2F_{7/2}$ and Yb^{3+}:$^2F_{5/2}$ (Fig., curves 4, 5).

Acknowledgements

The authors acknowledge financial support by the National Scholarship Programme of the Slovak Republic supporting the study stay of Dr. I. Sulym (Contract number 19862) at the Department of Inorganic Materials, Faculty of Chemical and Food Technology, SUT. The financial support of the Slovak Grant Agency for Science VEGA No. 1/0278/16, 1/0906/17 and 1/0527/18 are greatly appreciated.

Fractal approach to the analysis of the kinetics of the heterogeneous-catalytic reaction

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Surface of a catalyst usually has complex structure that can be described by the fractal geometry [1], particularly the fractal dimension (DF) can be used to characterize the surface properties of a solid catalyst and to quantity the surface characteristics. The fractal dimension of solids can be determined by different methods such as adsorption, small angle X-ray and neutron scattering, mercury porosimetry, electron microscopy, *etc*. Based on a purely geometrical consideration, recalculating a number of active sites for a catalyst with fractal geometry, it was shown a relation between the turnover number and the fractal dimension [2]. Many experiments show an effect of the fractal structure of a catalyst on catalytic reactions.

We develop a theoretical approach establishing a relation between the fractal dimension of porous catalyst and the rate constant of heterogeneous catalytic processes. To verify theoretical results, we perform a study of the CO oxidation on various nanoporous materials, which are characterized by different fractal dimension in the range between 2 and 3.

We establish a relation between the activation energy and the activation entropy of the activated complex of heterogeneous catalytic reaction and fractal dimension of porous catalyst. It was demonstrated that the total energy, the activation energy and the activation entropy increase with increasing the fractal dimension if other parameters of a system are constant.

A good correspondence between the fractal approach to catalysis by porous materials, and experimental results illustrates that the approach can be used to catalysis by nanoporous materials with similar chemical nature, namely, with similar active sites. These materials are widely used not only as catalysts but also as catalyst supports or sorbents. They also depend strongly on morphology of their surface, excess surface energy, surface inhomogeneity, and other characteristics, which are related to surface morphology. In many cases, mainly these factors affect significantly the reaction rate. Approach we have developed gives a relation between the rate constant of heterogeneous catalytic process and the surface fractal dimension of a catalyst. The approach is verified by experimental study of the CO oxidation on various nano and mezoporous materials.

1. W.G. Rothschild, Fractals in Chemistry, John Willey & Sons, Inc., New York, 1998.
2. J.J. Carberry, J. Catalysis **114** (1988) 277.

Silicates glass and glass-ceramics activated RRE-ions are promising materials for scintillation and luminescence's applications

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The glasses and glass-ceramics based on stoichiometric compounds with composition $xMO–ySiO_2$ (M = Mg, Ba, Ca, Sr; x, y = 1, 2, 3) were obtained in present work. Synthesis conditions (glass transition temperature), crystallization ability and luminescence properties of obtained glasses depend on the $MO:SiO_2$ ratio. Tendency for scintillation for stoichiometric compounds in $BaO–SiO_2$:Ce system was established. The highest light yield was registered for glass-ceramics with composition $BaO–2SiO_2$:Ce ($\lambda_{scint.}$ = 440 nm). Radiation hardness for these compounds has been studied. Possibility of activating of $BaO–SiO_2$ system by Ce^{3+}, Eu^{3+} and Tb^{3+} ions was demonstrated (Fig.). The compounds in the system $CaO–SiO_2$:Ce are characterized by absence of scintillation at saving high photoluminescence intensity. The bands of excitation luminescence at 340 nm and luminescence at 450 nm are making these compounds promising for applying as a luminescence shifter in combination with CeF_3 scintillation crystals.

a *b* *c*

Fig. Developed glass ceramics samples obtained with different RE activators (*a* – Ce^{3+}, *b* – Tb^{3+}, *c* – Eu^{3+}) at excitation with 390 nm LED light

Acknowledgements
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Preparation of SOD type zeolite from perlite

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Previously, the synthesis of LTA type zeolites from Georgian natural clinoptilolite was described [1], while the SOD type zeolite was an intermediate product. Sodalite was considered as a potentially interesting containment matrix for chloride salts wastes [2] and as an effective adsorbent for heavy metal disposal [3], Na-sodalite was crystallized from kaolinite, sodium chloride, and sodium hydroxide mixture [2], and sodalite was prepared by alkali fusion-desilication-hydrothermal method using fly ash as raw material [3].

Preliminary dispersed (<40 μm) and activated by acid treatment amorphous volcanic glass perlite from the Paravani lake deposit (Southern Georgia) has been used as a raw material and as a source of Si and Al for the hydrothermal synthesis of the SOD type zeolite materials under following conditions: reaction mixture $Na_2O:Al_2O_3:SiO_2:H_2O=4:4:1:22$, temperature 95-105°C, crystallization duration 7 hrs.

According to the data of elemental analyses (Spectromom 381L, Perkin-Elmer 300), chemical composition of prepared samples, Si/Al = 1.05(5), Si/O = 4.0(2), Na/Al=0.97(5), corresponds to the IUPAC formula of sodalite. The FTIR spectra (Perkin-Elmer 10.4.2, KBr pellet) testifies the zeolite nature of obtained material. Experimental X-ray powder diffraction pattern (DRON-4 employing the CuK_α line) is in a good agreement with measured powder pattern for hydroxy-sodalite from Database of Zeolite Structures of the International Zeolite Association, showing high intensity peaks at 2Θ = 14.1° (60%, *hkl*=110, *d*=6.27Å), 24.6° (100%, 211, 3.6Å), 32° (98%, 310, 2.77Å), 35.1° (78%, 222, 2.52Å), and 43.3° (35%, 411, 2.05Å), as well as comparatively weak peaks at 2Θ = 20° (16%, 200, 4.43Å), 28.5° (21%, 220, 3.1Å), 38° (14%, 321, 2.33Å), and 48.2° (12%, 332, 1.84Å). Morphology of crystals and their sizes have been determined from SEM images (Jeol JSM6510LV with Oxford Instruments X-Max 20 analyzer for EDS), porosity parameters from BET and BJH isotherms (ASAP-2020).

Preparation of cationic forms for obtained zeolite material and study of their properties are in progress.

1. N.M. Dolaberidze, V.G. Tsitsishvili, N.A. Mirdzveli, M.O. Nijaradze, Chem. Phys. Techn. Surf. **8** (2017) 346.
2. H. Rabiller, F. Bart, JL. Dussossoy, T. Advocat, P. Perouty, D. Rigaud, V. Gori, C. Mazzocchia, F. Martini, in: ATALANTE 2004: Advances in future nuclear cycles, Nimes (France), 2004.
3. L. Luo, H. Zhang, J. Yang, Procedia Env. Sci. **31** (2016) 605.

Influence of solid and liquid hydrophobic compounds on characteristics of water located in an adsorption layer of a hydrophilic component of the system

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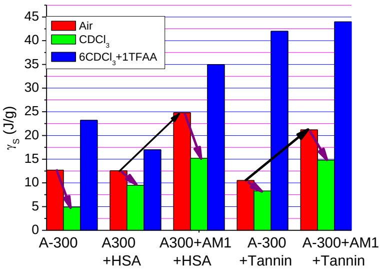
Previous investigations showed that hydrophobic modified silicas added to hydrated hydrophilic systems can affect the temperature behavior of bound water. It is possible both increase and decrease of temperatures of melting, evaporation and freezing of bound water. The reasons of these phenomena are not clear in detail. Therefore, the aim of this study was evaluate the influence of solid and liquid hydrophobic compounds on bonding of water in composite systems based on nanosilica A-300 and such biogenic substances as human serum albumin (HSA) and pharmaceutic tannin. According to data of low-temperature ^{1}H NMR spectroscopy for all systems studied, replacement of the air medium by weakly polar chloroform leads to a significant diminution of bonding energy of water interacting with a surface (Fig.). The maximal effect is observed for hydrated bare silica since the value of γ_S decreases from 12.7 to 4.9 J/g. This effect is due to a strong diminution of the amount of strongly bound water. The driving force of restructurization of bound water corresponds to a decrease in the contact area between immiscible liquids. Chloroform can displace water from narrow voids between nanoparticles to form larger structures in larger voids. Therefore, contribution of relatively small water cluster sat $R < 7$ nm decreases, but contribution of water domains at $R > 10$ nm increases. In the case of the HSA solution (with the same content of water), this effect is much smaller because water remains in state bound to hydrophilic parts of HSA, but chloroform can be bound to hydrophobic pats of the albumin. This reduces direct contacts between the bound liquids.



There is an additional general end characteristic for nanosilica with bound HSA or tannin that corresponds to an increase in water bonding for a mixture of hydrophilic and hydrophobic (1:1) silicas instead of pure hydrophilic one. This effect can be similar to effects observed for “dry water”; i.e., a hydrophilic component interacts with water, but a hydrophobic component interacts with chloroform. Additionally, mechanical loading (upon preparation of the mixture) results in changes in the texture of the complex powder. A decrease in the size of voids with parallel increase in the volume of these voids causes stronger bonding of larger amounts of water than in the case of hydrophilic silica alone.

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Surfactants and natural polymers in flocculation process

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Last time natural polymers became a subject of intensive research. This is caused by the unique complex of environmental and physicochemical properties: biodegradability, playback of the raw material base, complexing ability, compatibility with living tissues without toxicity.

The aim of our researches was to study the role of complexes based on polymers in solution with the addition of anionic and cationic surfactants (sodium alkylsulfates and alkylammonium chlorides) in flocculation process.

There were researched some parameters of the macromolecular chains which characterized the process of associates' appearing. As a result of the formation of associates, the root mean square radius of gyration is reduced. Researches had shown that pre-association of the surfactants with chitosan and alginic acid salts leads to increase its sorptive and flocculating capacity. This is confirmed by our study of surface activity and viscosity systems. For systems surfactant - chitosan, surface tension decreased to $30 \cdot 10^{-}3$ N/m and for systems surfactant-alginic acid salts - to $45 \cdot 10^{-}3$ N/m. Emerging associates are more hydrophobic. The effect becomes stronger with increasing length of the hydrocarbon surfactant radical from 8 to 16 carbon atoms, as well as in time. This is due not only to the process of association, but with the change in the conformation of macromolecules.

The results of IR-spectroscopic research of samples of polymers and surfactants confirmed there was no chemical interaction in the researched systems. The formation of the hydrogen bonds between the functional groups of chitosan and surfactants is observed.

Flocculation ability chitosan and alginic acid salts in presence surfactants were studied in suspensions of kaolin. It was shown, that natural flocculants are more effective than synthetic. The flocculation causes either because of the formation of polymer "bridges", or because of neutralization of the surface charge of the particles. The formation of polymer-colloid nanoscale complexes polyelectrolytes-surfactants in solution is making a positive contribution to improving the efficiency of flocculation of suspensions. In this case, the degree of aggregation particles increases and accelerates phase separation process.

Mechanical and protective properties of composite nickel coatings

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Electrodeposition can be used in order to prepare nanocomposite coatings made of nanoparticles dispersed into a metallic matrix, onto a metallic substrate. Including diamond nanoparticles into a metallic matrix can take advantage of the diamond properties, especially of its hardness and inertness in many chemical media [1, 2]. Still, the proper control of the electrodeposition parameters is a must in order to obtain the best microhardness and corrosion behavior of such nanocomposite coating. This paper proposes that pulse electrodepositiont method by frequency 50 Hz and the duty cycle 50 be used in order to prepare Ni/diamond nanocomposite coatings with the best microhardness and best corrosion resistance.

It was found out that the diamond nanoparticles content increases by employing pulse electrodeposition from 2.24 to 4.45 wt.%. The experimental results proved that the microhardness and the roughness (Fig.) of the Ni/diamond nanocomposite coatings were strongly influenced by the presence of the nanoparticles as compared to pure nickel coatings. , The microhardness of the nanocomposite coatings increased from 1800 to 3200 MPa

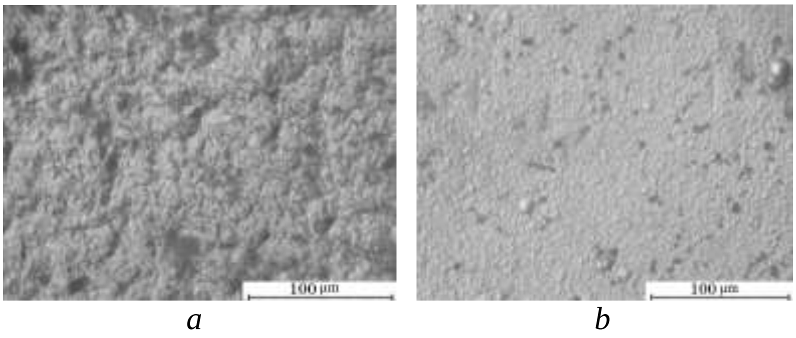

Fig. Surface morphology of composite nickel coatings: *a* – D.C.; *b* – P.C.

Established that the corrosion resistance was improved by a decrease of the grain size onto the coating, since into finer grain coating the passivation was better. Average corrosion penetration decreases from 0.014 to 0.005 mm/year, number of pores per 1 cm^2 decreases from 24 to a practical absence.

1. G.K. Burkat, T. Fujimura, V.Yu. Dolmatov, E.A. Orlova, M.V. Veretennikova, DRM. **14** (2005) 1761.
2. L. Wang, Y. Gao, Q. Xue, H. Liu, T. Xu, Mater. Sci. Eng. A. **390** (2005) 313.

Synthesis route to the strychnos-type alkaloids

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A novel approach to prepare the core structure of strychnos-type alkaloids is described. The strategy is based on a Fischer indole synthesis. It is known to have a wide variety of applications including the synthesis of indole ring, often present as the framework in the total synthesis of natural products an indole alkaloid. In this study, we are trying to constitiue the tetracyclic framework of strychnos-type alkaloids as well as the ABDE substructure of the strychnos alkaloid family, which is applied to the total synthesis of biologically active natural products and some other complete targets. This important complexity-generating transformation provides the tetracyclic core of many indole monoterpene alkaloids in only three steps from commercially available starting materials and played a key role in the short syntheses of uleine dasycarpidone, deethyltubifolidine, tubifolidine. The aim is this study is to provide an overview of the synthetic methods published 1960 for constructing the 1,5-methanoazocino[4,2-*b*]indole framework of strychnos-type alkaloids with more complex structures.

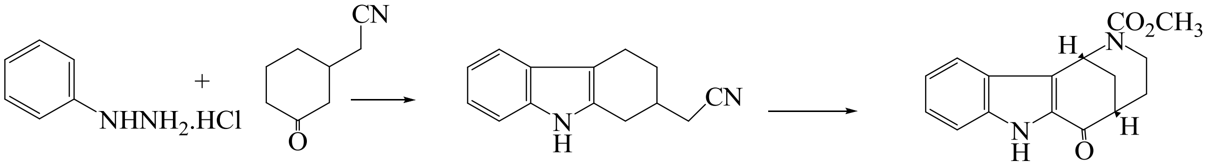

Fig. Synthetic strategy

1. E.J. Saxton, Recent progress in the chemistry of the monoterpenoid indole alkaloids, Nat. Prod. Rep. **14** (1997) 559.
2. N. Uludag, G. Serdaroglu, J. Mol. Struct. **1155** (2018) 548.
3. S. Patir, N. Uludag, Tetrahedron, **65** (2009) 115.
4. N. Uludag, R. Yilmaz, O. Asutay, N. Colak, Chem. Heterocycl. Compd. **52**, (2016) 196.
5. N. Uludag, M. Yakup, Org. Prep. Proc. Int. **47** (2015) 454.

A new route to the deethylaspidospermidine

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Aspidosperma alkaloids have a pentecyclic skeleton (ABCDE) imbedded in an indoline structure. These molecules are known to have significant biological activities, and class includes the antitumor agents vincristine and vinblastine. Deethylaspidospermidine is the parent structure for *Aspidosperma* alkaloids and as such, has been the primary target for most of the approaches towards *Aspidosperma* alkaloid synthesis. Many synthetic approaches [1-5] have been attempted, including the intramolecular cascade transannular cyclization approach, the palladium(0)-catalyzed Ullmann cross coupling approach, and the oxidative Hosomi–Sakurai approach. Although, significant efforts have been devoted to synthesize deethylaspidospermidine they have been limited. Therefore, we have decided to seek a shorter and more efficient route to the pyrido[3,2-*c*]carbazole, a key feature in *Aspidosperma*, alkaloids such as deethylaspidospermiden, ibophylidine and aspidospermidine. In this work we previously report a new synthetic strategy for the total synthesis of the alkaloid 20-deethyl-4-demethyldasycarpidone featuring an intramolecular cyclization mediated by 2,3-dichloro-5,6-dicyanobenzoquinone(DDQ), and thoroughly intramolecular an aldol reaction. We now report an extension of this approach that leads to the total synthesis of deethylaspidospermidine.

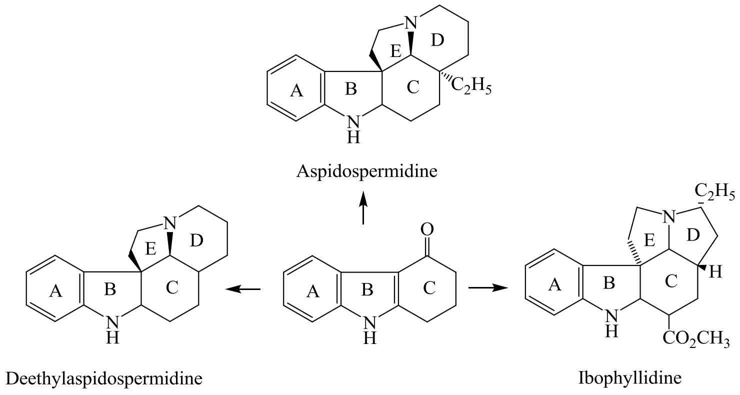

Fig. Deethylaspidospermidine and aspidosperma-type alkaloids

1. M. Toyota, M. Ihara, Nat. Prod. Rep. **15** (1988) 327.
2. J. E. Sakton, Nat. Prod. Rep. **11** (1994) 493.
3. E. Wenkert, J. S. Bindra, B. Chauncy, Synt. Commun. **2** (1972) 285.
4. N. Uludag, T. Hokelek, S. Patir, J. Heterocycl. Chem. **43** (2006) 585.
5. S. Patir, N. Uludag, Tetrahedron. **65** (2009) 115.

The application of kinetic models to the description of sorption of strontium ions onto inorganic sorbents

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In this work the sorption of strontium ions by zirconium silicate, titanium phosphate, zeolite and some other crystal or amorphous inorganic sorbents from aqueous solutions was investigate in the batch mode. The sorption of Sr^{2+} ions strongly depends on time of interaction between solution and surface of sorbents. The limits of the application of kinetic models to the description of sorption processes are considered.

Elovich kinetic model, diffusion kinetic model, Lagergren's pseudo first and pseudo second order kinetic models [1-5] were applied to the experimental data.

The most of all of sorption systems 'solution of strontium – inorganic sorbent', are well fitted by Lagergren's pseudo second kinetic model.

A special attention is paid to possible theoretical grounds of the most commonly applied mathematical expression, such as pseudo first and pseudo second order equation. Simple theoretical considerations based on some fundamental theories suggest that these two formulae do not correspond to any specific physical model [1].

However, the Lagergren's coefficients have a certain physical meaning, and their relation is the parameter *в* in the Langmuir equation. The same opinion is expresses by the authors of the publications [1, 2]. It is very interesting, because the parameter *в* is related to the thermodynamic characteristics of the sorption process, according to the author's [3] data.

1. W. Plazinski, W. Rudzinski, A. Plazinska, Adv. Colloid Interface Sci., **152** (2009) 2.
2. S. Azizan, J Colloid Interface Sci., **276** (2004) 47.
3. A. Adamson, Physical Chemistry of Surfaces, Mir: Moskow, 1979.
4. Y.-Sh. Ho, Scientometrics, **59** (2004) 171.
5. N.R. Villarante, A.P. Bautista, D.E. Sumalapao, Oriental Journal of Chemistry, **33** (2017) 1111.

The effect of Pluronic on gold nanoparticles synthesized in the presence of tryptophan

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In our works we promote essential amino acid tryptophan as a nontoxic agent for silver/gold nanoparticles (NPs) preparation. The use of tryptophan as a reducing agent of metal ions and a particle stabilizer resulted in producing of stable metal colloid that possess low toxicity and anticancer effect [1-4]. The further use of Ag/Au NPs for medical examination requires highly concentrated metal colloids. In this study we developed synthetic procedure to increase metal concentration in colloid without loss of stability and nanodimension of particles. For this purpose we used polymer Pluronic F68.

Polymer allowed to increase the concentration of nanosized gold in 40 times up to $C_{\mathrm{Au}} = 4 \cdot 10^{-3}$ M that corresponded to 0.8 mg/ml of gold. At such high concentrations of metal gold colloids are very dark liquids, almost indistinguishable by color. But specific bright color due to absorption of localized surface plasmon resonance (LSPR) of gold appeared after colloid dilution. The position of LSPR band was located at 528 nm and was typical for Au nanoparticles.

The effect of Pluronic on size and stability of gold NPs, as well as their aggregation process, was analyzed. The narrowing of LSPR band of gold in time due to aggregation in Au/Trp system was not observed in case of Au/Trp/pluronic. According to dynamic light scattering data polymer fixed particles with the average size of 5 nm (number/volume basis), compare to 10-20 nm for Au/Trp system without polymer. At the same time it promoted the formation of twice larger aggregates of NPs of 200-400 nm (intensity basis), that supposedly are localized along polymeric chain.

1. I.O. Shmarakov, Iu.P. Mukha, V.V. Karavan, O.Yu. Chunikhin, M.M. Marchenko, N.P. Smirnova, A.M. Eremenko, Nanobiomedicine. **1** (2014) 01.
2. Iu. Mukha, N. Vityuk, O. Severynovska, A. Eremenko, N. Smirnova, Nanoscale Res. Lett. **11** (2016) 101.
3. Iu. Mukha, N. Vityuk, G. Grodzyuk, S. Shcherbakov, A. Lyberopoulou, E.P. Efstathopoulos, M. Gazouli, J. Nanosci. Nanotechnol. **17** (2017) 8987.
4. I. Shmarakov, Iu. Mukha, N. Vityuk, V. Borschovetska, N. Zhyshchynska, G. Grodzyuk, A. Eremenko, Nanoscale Res. Lett. **12**:333 (2017).

Effect of mechanical and ultrasonic treatment of nanosilica aqueous suspension on gelatin adsorption

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Used in medicine as aqueous suspensions and gels, fumed nanoscale silica with a specific surface area of 300 m^2/g consists of spherical particles with a diameter of 9-10 nm. Such nanosilica particles by means of hydrogen bonds between the surface silanol groups form aggregates with a diameter of 100-200 nm, which can be combined into micron-sized agglomerates. Hypothetically, it can be assumed that such a hierarchical structure of nanosilica will be influence on the adsorption of various molecules, especially those with high molecular weight on the sorbent surface.

Therefore, the aim of the work was to study the influence of various methods of physical impact, which lead to the destruction of aggregates and agglomerates, on adsorption of gelatin on the surface of nanosilica from an aqueous solution.

Adsorption of gelatin on the surface of nanosilica was carried out under static conditions at $t = 16 \pm 1$ °C, pH = 4.7, $\tau = 1$ hour. The suspension was then centrifuged: $\omega = 7000$ rpm, $\tau = 10$ min. The concentration of nanosilica in the suspension was the same (1% by weight). The initial concentration of gelatin was 0.6% by weight. Previously, it has been found that at such concentrations a monolayer of gelatin is formed. The physical effect on the suspensions was carried out by stirring in a paddle mixer ($\omega = 1000$ rpm, $\tau = 10$ min) and in a ball mill ($\omega = 60$ rpm, $\tau = 10$ min), sonication ($\tau = 10$ min). Control – manual stirring with a glass rod ($\tau = 1$ min). Two treatment options were used: 1) the suspension was first treated, and then gelatin was added; 2) gelatin was first added to the suspension, and then the resulting mixture was processed.

No.	pH	glass rod	paddle mixer	ball mill	sonication
1	4.7	222	264	310	272
2		220	284	320	240

The data obtained show that the physical effect on the aqueous dispersion of nanosilica leads to a certain increase in gelatin adsorption. The adsorption value does not depend on the sequence of such treatment. It is concluded as a result of physical influence, the structure of the nanocomposite changes.

Some features of high-temperature Brownian ratchets governing by small harmonic fluctuations of potential energy

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It is known that fluctuations of characteristics of nanoscale systems, under the broken symmetries of detailed balance and reflection, can cause the ratchet effect [1]. A spatially harmonic signal as a source of perturbation of a stationary spatially periodic asymmetric potential (formed, e.g., by substrates, layers, microtubules, and other tracks along which a particle moves) is promising for controlling the motion direction and efficiency of ratchets, because signals of this type are easily obtained and widely used in applications.

The present study concerns nanoscale transport induced by potential energy fluctuations with a sinusoidal coordinate dependence. We consider a stochastic ratchet with the potential energy $U(x,t)= u(x)+\sigma(t)w(x)$ governed by the small harmonic fluctuations, $w(x)=w_0\cos 2\pi(x/L-\lambda_0)$ of the periodic stationary component $u(x+L)=u(x)$, L is the period. We are based on the general analytical expression for the average ratchet velocity [2]

$$\langle v\rangle = -L(\beta D)^2\int_0^L dx\rho_+^{(0)}(x)w'(x)\int_0^L dyG(x,y)\frac{\partial}{\partial y}w'(y)\rho_-^{(0)}(y)\,;\ \rho_\pm^{(0)}(x)=e^{\pm\beta u(x)}\Big/\int_0^L dxe^{\pm\beta u(x)}\,,$$

$\beta=1/k_BT$, D is the diffusion coefficient, $G(x,y)$ is the Laplace representation of the Green's function for diffusion in the unperturbed potential $u(x)$. The function $u(x)$ is taken as a sawtooth one with the amplitude u_0. The high-temperature approximation (HTA) allows analytical analysis, while, out of it, we use numerical treatment. We analyze a response of $\langle v\rangle$ on the phase shift λ_0 of the control signal $w(x)$ relative to $u(x)$. While within HTA $\langle v\rangle$ is multiplicative in system parameters [2], the regime beyond HTA violates the multiplicativity. For certain fixed values of the asymmetry κ of $u(x)$, an increase in u_0 leads to an increase/decrease in the size of the region of positive/negative values of $\langle v\rangle$. Thus, there may exist a regime of u_0 values in which the negative current will be totally suppressed. The role of competition between κ and λ_0 in magnitude and direction of $\langle v\rangle$ is studied as well as the temperature behavior of stopping points. The strategy of the choice of optimal motor parameters is discussed.

1. D. Cubero, F. Renzoni, Brownian Ratchets: From Statistical Physics to Bio and Nano-motors, UK: Cambridge University Press, 2016.
2. U.A. Vysotskaya, I.V. Shapochkina, V.M. Rozenbaum *et al.*, Chemistry, Physics and Technology of Surface. **8** (2017) 299.

Long-term stability of solid acid fuel cell electrodes

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Solid acid fuel cells are a relatively new type of fuel cells with a midrange operating temperature of 240°C [1]. This temperature range provides numerous advantages and solid acid fuel cells with a very promising initial activity have already been reported in the past years [2]. However, the long-term stability remains a challenge. In this work, we investigated the degradation behaviour of thin film and porous electrodes using impedance spectroscopy, scanning electron microscopy, X-ray diffraction and constant voltage measurements. We found out, that the used electrolyte CsH_2PO_4 changed its appearance close to the current collectors after a 24 h measurement with an average current density of 30 mA/cm² going through the cell. Combining the results of all conducted measurements, we suggest that the observed change is caused by current induced thermal degradation.

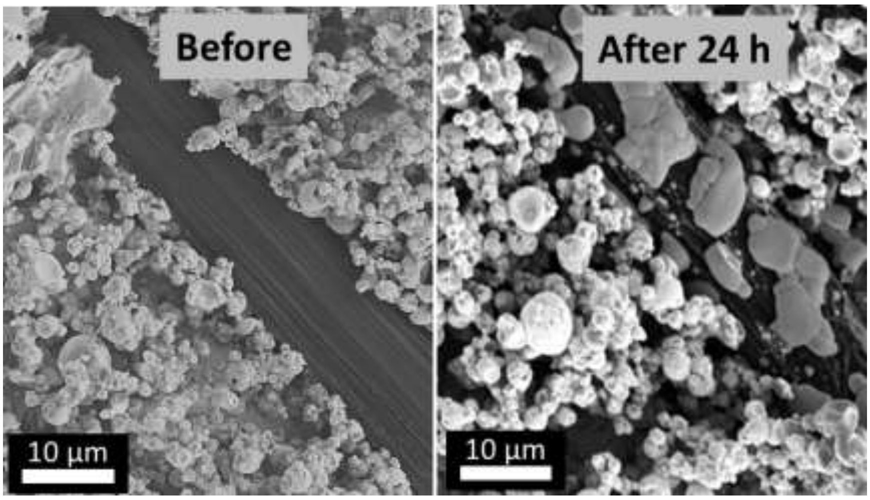

Fig. Micrograph of the electrolyte CsH_2PO_4 close to the current collector before and after a 24 h measurement. The degradation of the nearby electrolyte afterwards is clearly visible

1. D.A. Boysen, T. Uda, C.R.I. Chisholm, S.M. Haile, Science. **303** (2004) 68.
2. A.B. Papandrew, R.A. Elgammal, M. Tian, W.D. Tennyson, C.M. Rouleau, A.A. Puretzky, G.M. Veith, D.B. Geohegan, T.A. Zawodzinski, J. Power Sources. **337** (2017) 145.

Adsorption of silver ions by hydroxyapatite-alginate microspheres

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Hydroxyapatite (HA) was chosen as a basic component for biomaterials due to its high sorption capacity to metal ions, biocompatibility, osteoconductivity and thermodynamic stability. HA synthesis was following:
$10Ca(NO_3)_2{\cdot}4H_2O + 6(NH_4)_2HPO_4 + 8NH_3{\cdot}H_2O \rightarrow Ca_{10}(PO_4)_6(OH)_2 + 20NH_4NO_3 + 46H_2O$.
Obtained HA was washed three times with distilled water and filtered. HA slurry was mixed with 1.5 % sodium alginate (Alg) solution in relation 1:1. Then HA-Alg mixture was added dropwise into 0.1 M $CaCl_2$ solution, washed and immersed into 0.1 M $AgNO_3$ solution. Morphology of obtained microspheres after 24 h immersion is given in the Fig.

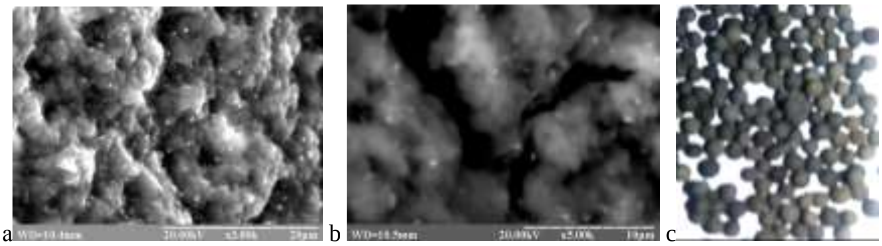

Fig. HA-Alg microspheres obtained in $CaCl_2$ solution and immersed on 24 h into 0.1 M $AgNO_3$ solution. SEM images of *a* - surface, *b* - inside pore, *c* - general view of microspheres

Then the solutions were filtered and concentrations of Ag^+ ions in the filtrate were determined by nephelometric analysis (Table).

Table. Adsorption of Ag^+ ions by HA-Alg microspheres (m=1 g) at 36ºC

Sample number	1	2	3	4	5	6
Time period, min	10	60	120	240	600	1440
Concentration of Ag^+ in filtrate, mg/mL	10.70	9.77	6.24	5.14	4.65	4.12
Ag^+ ions concentration, mg/g.	1.00	10.24	45.69	56.00	61.38	66.65

After 60 and 120 min silver was adsorbed only by the surface layer but after prolonged contact it was absorbed completely. More than 60 % of Ag^+ ions from solution are incorporated in HA structure. First the silver orthophosphate was formed and then it was destructed under UV-light with following formation of silver nanoparticles.

Hydrated properties of the composite system based on high-dispersed silica and *Amanita muscaria*

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Currently, fungi *Amanita muscaria* is used not only in folk medicine, but also in traditional medicine for the treatment of such serious diseases as epilepsy, atherosclerosis, varicose veins, *etc*. A promising trend in the use of *Amanita muscaria* for both internal and external applications may be its inclusion in the composition of nanocomposite systems based on highly dispersed silica A-300. At the same time, it can be expected that toxic substances that are bound with *Amanita muscaria* enzymes will not be desorbed from the composite system due to the high protein-sorbing ability of nanosilica, while bioactive substances of low and medium molecular weight will be delivered to the intestinal mucosa.

The purpose of this work was to study the water binding energy and the structure of water in fungi *Amanita muscaria*, the initial ones dried to a residual moisture of 120 mg/g and included in the composition of the nanocomposite with silica, after its wetting-drying to a bulk density of P_d = 200 mg/ml.

In the initial biomaterial of the fungus *Amanita muscaria*, almost all the water is in a bound state, however only 12% of water presents in the tissues of the fungus is strongly bound. The amount of weakly associated water is small and amounts to 25 mg/g, of which the majority also refers to loosely bound water. After the sample is dried, the fraction of strongly bound water increases to 30% in the aerial medium and up to 80% in the medium of $CDCl_3$. In this case, the interphase energy (σ_S) increases almost three times – from 3.4 to 10.3 J/g. Such a high growth of water binding energy is probably due to its transition from the clustered state in air to the state of a nanoscale two-dimensional film in a medium of $CDCl_3$. The difference in the value of σ_S determines the energy gain from such transformation.

It is shown that the water contained in the fungus or its composite with nanosilica can be in strongly and weakly associated states. The latter is stabilized by contact with a weakly polar medium, which simulates the hydrophobic part of phospholipid structures and the intestinal mucosa. It is suggested that in the body this effect will increase the bioavailability of the active substances desorbed from the composite system.

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Sorption of U(VI) ions by montmorillonite and organomontmorillonite modified by nanosized zero-valent iron

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Nanocomposite materials based on nanoiron display high characteristics for removal organic and inorganic toxicants from contaminated water [1]. However, disadvantages of materials based on nanoiron are the tendency of particles to aggregation and a high speed of oxidation. Therefore, montmorillonite was used as dispersed inorganic matrix for immobilization nanoiron particles on its surface. Surface organofilization was carried out for the purposeful regulation of hydrophobic and hydrophilic properties of the surface and it is expedient to study nanocomposite materials based on organofilized montmorillonite.

The iron-containing materials were synthesized on the basis of montmorillonite and organofilized montmorillonite. Organomontmorillonite was obtained by modifying the surface of montmorillonite by the cation surfactant hexadecyltrimethylammonium bromide. The synthesis of nano-dimension zero-valent iron was carried out by reduction of iron from salt $Fe_2SO_4 \cdot 7H_2O$ by the reducing agent $NaBH_4$. Mass ratio between the components of the nanocomposite materials was 1:4 Fe^0 to montmorillonite or organomontmorillonite.

It was shown that a monolayer of surfactant formed on the surface between structural packages of montmorillonite contributes to the formation of more dispersed particles of zero-valent iron. It was defined that the sorption characteristics of organomontmorillonite and montmorillonite modified with iron nanoparticles are significantly higher (326 and 301 μmol/g) than on the original mineral (75 μmol/g) and even on pure nano-dispersed iron (151 μmol/g) in relation to U(VI).

The obtained nanocomposite materials possibly can be used in innovative environmental technologies based on pumping aqueous dispersions of nanomaterial into contaminated layers of soil.

1. V. Tobilko, O. Makovetskyi, I. Kovalchuk, B. Kornilovych, Eastern-European Journal of Enterprise Technologies. **5** (2015) 34.

Non-Fickian diffusion in mesoporous media: adsorption induced

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The presence of the anomalous diffusion has been studied for various systems both theoretically and experimentally. However, the reasons of the anomalous diffusion induction remain scarce. Moreover, one global physical origin of the anomalous diffusion arousal does not exist. It is strongly individual for each particular case.

Here we report the experimental study of the methanol mass transfer in the mesoporous silica and alumina/zeolite H-ZSM-5 grains. We demonstrate that the methanol diffusion is characterized as a time-fractional for both solids. Methanol transport occurs in the super-diffusive regime, which is faster comparing to the Fickian diffusion. We show that the fractional exponents defining the regime of transport are different for each porous grain. The difference between the values of the fractional exponents is associated with a difference in the energetic strength of the active sites of the surface of the media of different chemical nature as well as the geometrical restrictions of the porous media. Increasing six-fold the pore diameter leads to 1.1 fold increase of the fractional exponent. Decreasing three-fold the methanol desorption energy results into the same increasing the fractional exponent. Our findings support that mainly the adsorption process, which is defined by the energetic disorder of the corresponding surface active sites, is likely to be the driving force of the abnormality of the mass transfer in the porous media. Therefore, the fractional exponent is a fundamental characteristic which is individual for each combination of the porous solid and diffusing species.

The impact of the adsorption on the fractional order is considerably higher comparing to the impact of the pore diameter. Therefore, the adsorption process is the main driving force for the arising of the nonlinear anomalies in the mass transfer kinetics in the energetically disordered geometrically restricted media.

Tetra-acid complexes of trimecaine

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Anesthetic preparation 2-diethylamino-N-(2,4,6-trimethylphenyl)-acetamide hydrochloride monohydrate (Tm·HCl) is one of the most generally used local anesthetics and peripheral analgesics in surgery, genecology and dentistry. It is white crystalline powder readily soluble in water and in ethanol; it is used as a local anesthetic, cardiac antiarrhythmic as well as for prophylaxis of sympathetic reaction during tracheal intubations. Increasing scientific evidence suggests that the purposeful synthesis and research of coordination compounds containing bio-metals and anesthesia drugs is interesting in the field of medical science and current pharmaceuticals.

We report the synthesis, structural and spectroscopic characterization of Trimecaine complexes. Protonation of ligands takes place in the water-ethanol solution of transit ion metal salt and Tm·HCl with various ratio, the complexes of empirical formula $(TmH)_2[MX_4]\cdot nH_2O$ (TmH-cationic form of the Trymecaine, M=Ni(II), Co(II), Cu(II), Zn(II), Fe(II), Sn(II), Cr(III); $X=Cl^{-1}$, NCS^{-1}) are formed. It should be also mentioned here that under test conditions, in parallel with the synthesis it has been conducted oxidation-reduction process and instead of Sn(II) we got compound $(TmH)_2[SnCl_6]\cdot H_2O$ containing Sn(IV).The composition and individuality of the complexes are determined by elemental analysis and melting temperature. Their solubility in water and organic solvents has been studied. In the compounds, the central ion coordination with acid ligands generates tetrahedral anion, while the ligands in the form of protonated cations remain in an outer coordination field. The study included the synthesis of new compound, the determination of its chemical composition, preparation of single crystals of Trimecaine and the target product, and finally their research by the X-ray diffraction method. Tm·HCI crystallizes in the rhombic space group Paac with a=28.999(5), b=11.190(3), c=10.573(3) Å, and Z=8, forming crystal structure, in which TmH^+ ions are united in infinite chains by intermolecular NH…CI…HN bonds, while water molecules connect chains by OH…CI…HO bonds. $(TmH)_2[SnCI_6]\cdot H_2O$ crystallizes in the rhombic space group $P2_12_12_1$ with a=10.745(1), b=14.199(2), c=26.166(3) Å, and Z=4, forming structure of molecular crystal with distorted $SnCI_6^{2-}$ octahedrons asymmetrically associated with water molecule and two TmH^+ ions by two CI…HO, O…HN, and bifurcated NH…2CI hydrogen bonds.

Gas-phase deposition of a cavitation-resistant coating based on boron carbide

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One of the problems, which leads to decrease in performance of nuclear power plants and capability utilization index, is the cavitation wear of distribution pipelines in steam generators. This results in severe localized destruction of structural materials. Typically such accidents appear in the sections of piping bends [1].

A solution to this problem is also possible through the protection of pipeline bend zones with coatings based on boron carbide. Boron carbide shows a high hardness, chemical inertness and low density, therefore this is a promising material to protect inner piping surface against cavitation wear.

This paper presents the results of studies produce boron carbide hydrogen reduction of boron trichloride BCl_3 and C_7H_8 toluene. Cavitation tests have shown that samples with a carbide-borne coating are 2.5 times less cavitation wear than austenitic steel (Fig.).

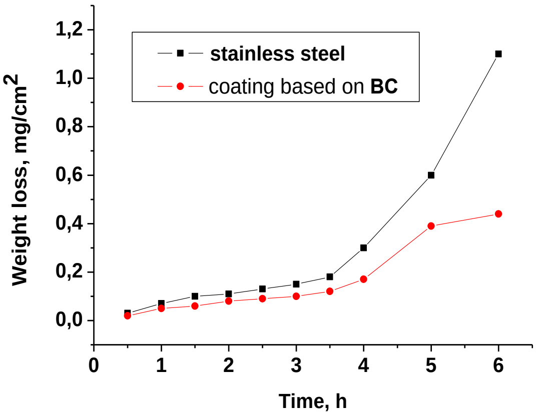

Fig. Cavitation wear of austenitic steel and austenitic coated steel

The experimental data obtained as a result of the research allow us to choose the parameters of the process of gas-phase deposition of coatings based on boron carbide, which will further facilitate the application of such coatings on the vortices of steam generators for protection against cavitation wear.

1. Erosion corrosion in power plant piping systems-calculation code for predicting wall thinning / W. Kastner, M. Erve, N. Henzel, B. Stellwag // International Atomic Energy Agency, Vienna (Austria). International Working Group on Reliability of Reactor Pressure Components; 93 p; Apr 1990; p. 49-59.

Organic-inorganic nanocomposites based on acrylates and 3-methacryloxypropyltrimethoxysilane

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Proton conductive membranes are the key elements of fuel cells, which are considered at present as effective and clean energy sources. It is very important to characterize the behavior of proton membranes in contact with water, since the presence of water in the membrane is a prerequisite for reaching high proton conductivity. It is well known that water resides in the hydrophilic domains and facilitates the transport of protons; however, too much water absorption results in the loss of mechanical stability.

In our study organic-inorganic membranes were synthesized by photoinitiated polymerization of acrylic monomers (acrylonitrile, acrylic acid, 3-sulfopropylacrylate potassium salt) in the presence of sol-gel precursor 3-methacryloxypropyltrimethoxysilane (MAPTMS). The results of water and methanol uptake studies for membranes with varied content of MAPTMS are shown in Fig. As one can see, the water uptake of the membranes gradually decreases with the increase of precursor content. In addition formation of hybrid system in nanocomposite membrane enhances the membrane stability [1].

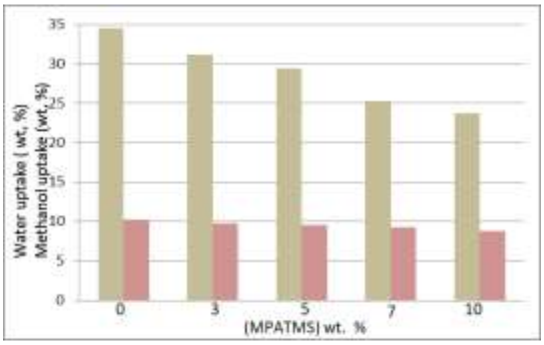

Fig. Water and methanol uptake of the membranes with different precursor content measured at 50 °C

Methanol uptake for investigated membranes is smaller and decreases for membranes with higher MAPTMS content, indicating that MAPTMS moieties may interfere with methanol permeation, thus facilitating proton transport through the sulfonic acid groups.

1. Y.-H. Su, Y.-L. Liu, Y.-M. Sun, Y.-L. Lai, D.-M. Wang, Y. Gao, B. Liu, M.D. Guiver, J. Membrane Sci. **296** (2007) 21.

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