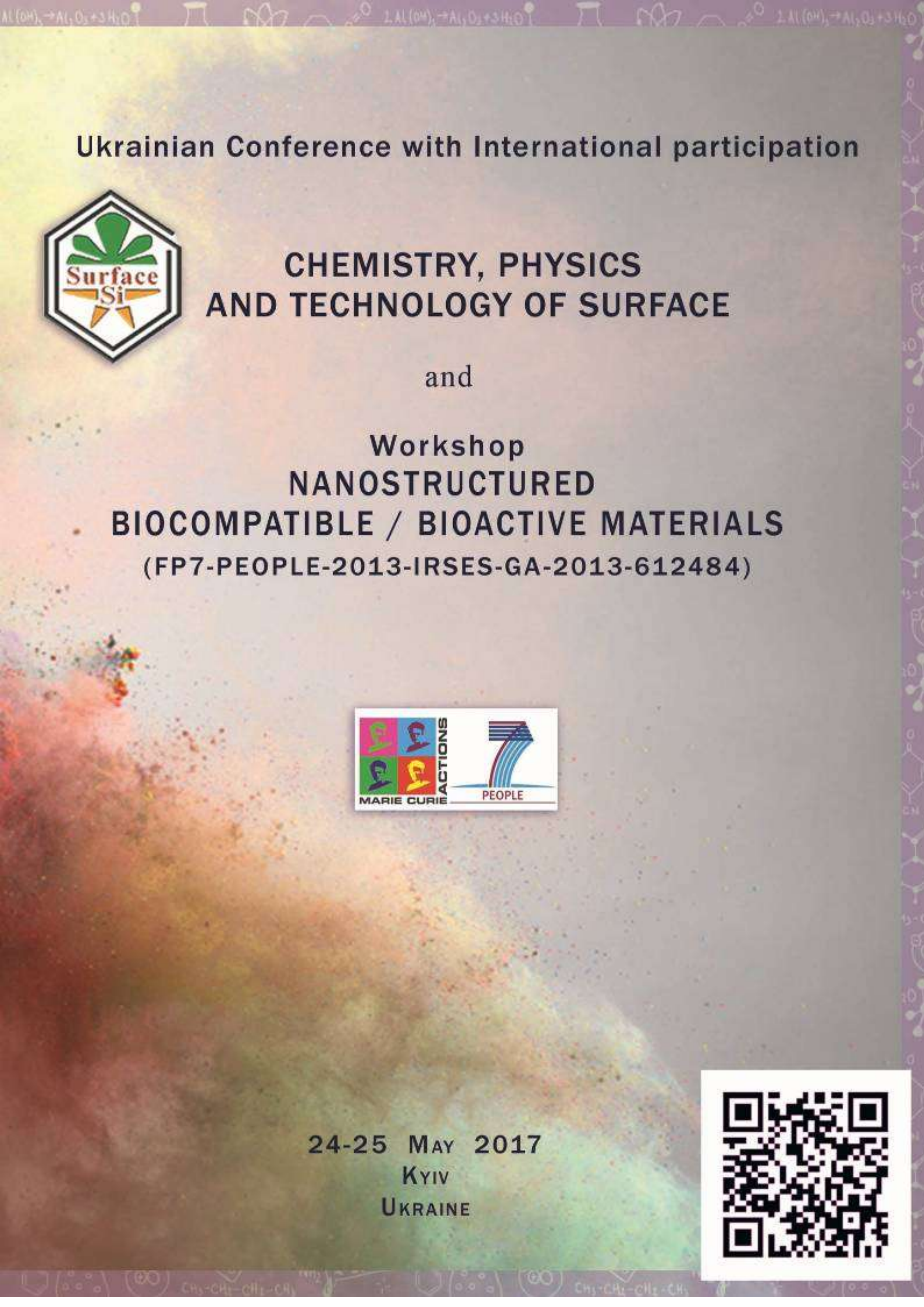

Ukrainian Conference with International participation

CHEMISTRY, PHYSICS AND TECHNOLOGY OF SURFACE

and

Workshop

NANOSTRUCTURED BIOCOMPATIBLE / BIOACTIVE MATERIALS

(FP7-PEOPLE-2013-IRSES-GA-2013-612484)

24-25 May 2017
Kyiv
Ukraine

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

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Book of abstracts

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Матеріали Всеукраїнської конференції з міжнародною участю «Хімія, фізика і технологія поверхні» і семінару «Наноструктуровані біосумісні / біоактивні матеріали» – Київ, 2017. – 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. Збірник призначено для наукових та інженерно-технічних працівників і студентів. Тези доповідей подано в авторській редакції.

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Conference Program

May 24, Wednesday

9:00 – 9:45 Registration of participants

10:00 – 10:10 Opening of the Conference in the Chuiko Institute of Surface Chemistry of NAS of Ukraine

Academician of NAS of Ukraine, Professor M. Kartel

Oral Session 1
Chair: *Professor M. Kartel*

10:10 – 10:35 **V.V. Turov**, T.V. Krupskaya, A.P. Golovan, L.S. Andriyko, M.T. Kartel. **A binding of water by cellulose matrix of medicinal plants and nanosilica (on the sample of *Hibiscus sabdariffa*)** *(Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv).*

10:35 – 11:00 N.S. Voloshina, L.N. Ognichenko, V.E. Kuz'min, **G.L. Kamalov**. **Structural factors of crown ethers interaction with aerosil surface** *(A.V. Bogatsky Physico-Chemical Institute, NAS of Ukraine, Odessa).*

11:00 – 11:20 coffee break

Oral Session 2
Chair: *PhD (Chem.) Yu. Bolbukh*

11:20 – 11:40 **A.W. Marczewski**, A. Deryło-Marczewska, M. Sęczkowska. **Simple models and equations of adsorption kinetics in practical application** *(Faculty of Chemistry, Maria Curie-Skłodowska University, Lublin, Poland).*

11:40 – 12:00 **A. Derylo-Marczewska**[1], M. Blachnio[1], A.W. Marczewski[1], T.M. Budnyak[2], V.A. Tertykh[2]. **Adsorption properties of chitosan-silica composites towards selected dyes** *([1]Faculty of Chemistry, Maria Curie-Sklodowska University, Lublin, Poland, [2]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv).*

12:00 – 12:15 **Ie.V. Dukhopelnikov**, E.G. Bereznyak, N.A. Gladkovska, D.A. Pesina, A.A. Herus. **Interaction of magnetite nanoparticles with negatively charged dyes** *(O.Ya. Usikov Institute for Radiophysics and Electronics NAS of Ukraine, Kharkiv).*

12:15 – 12:30 L.M. Soldatkina, **M.A. Zavrichko**. **Cetylpyridinium bromide-modified corn stalks for removal of Acid Red from aqueous solution** *(Odessa I.I. Mechnikov National University, Ukraine).*

12:30 – 12:45 L.M. Soldatkina, **V.O. Novotna**. **Adsorption removal of anthocyanins from red cabbage extracts by bentonite: statistical analysis of main and interaction effects** *(Odessa I.I. Mechnikov National University, Ukraine).*

12:45 – 13:00 **L.N. Ponomarova**[1], Yu.S. Dzyazko[2], Y.M. Volfkovich[3], V.E. Sosenkin[3]. **Organic-inorganic ion exchangers based on the strongly and weakly acidic polymeric matrices** *([1]Sumy National Agrarian University, Ukraine, [2]V.I. Vernadskii Institute of General and Inorganic Chemistry, NAS of Ukraine, Kyiv, [3]A.N. Frumkin Institute of Physical Chemistry and Electrochemistry of the RAS, Moscow).*

13:00 – 13:15 Z.Yu. Bunina[1,2], K.Yu. Bryleva[1,2], K.M. Belikov[1,2]. **Sorption performance of ethylene glycol dimethacrylate and methacrylic acid copolymers with different cross-link ratio towards rare earth elements** *([1]State Scientific Institution "Institute for Single Crystals", Kharkiv, [2]Faculty of Chemistry, V.N. Karazin Kharkiv National University, Ukraine).*

13:15 – 14:00 break

Oral Session 3
Chair: PhD (Chem.) O. Kazakova

14:00 – 14:20 V.E. Kuz'min[1], L.N. Ognichenko[1], I.F. Burdina[2], N.G. Sizochenko[3]. **Features of inorganic nanoparticles modelling. Nano-QSAR for cytotoxicity of metal oxides** *([1]A.V. Bogatsky Physico-Chemical Institute, NAS of Ukraine, Odessa, [2]Odessa National Medical University, Ukraine, [3]Interdisciplinary Center for Nanotoxicity, Jackson State University, USA).*

14:20 – 14:40 A.N. Herega, Yu.V. Kryvchenko. **Concept of nearest neighborhood at the percolation model of surface defects** *(Odessa National Academy of Food Technologies, Ukraine).*

14:40 – 14:55 I. Malinowska[1], **M. Studziński**[1], H. Malinowski[2]. **The influence of static magnetic field on silica gel free interphase energy** *([1]Planar Chromatography Department, Chair of Physical Chemistry, Faculty of Chemistry, Maria Curie-Skłodowska University, Lublin, Poland, [2]Joint Institute of Nuclear Research, Vexler and Baldin Laboratory of High Energy Physics, Dubna, Russia).*

14:55 – 15:10 V.S. Farafonov, A.V. Lebed, N.O. Mchedlov-Petrossyan. **Localization of the standard Reichardt's indicator in micelles of ionic surfactants from MD simulations** *(Department of Chemistry, V.N. Karazin Kharkiv National University, Ukraine).*

15:10 – 15:25 O.D. Kochkodan, R.S. Zhyla, T.S. Semenenko. **Bulk and surface properties of binary mixtures of surfactants** *(National University of Life and Environmental Sciences of Ukraine, Kyiv).*

15:25 – 15:40 N.M. Permyakova[1], T.B. Zheltonozhskaya[1], M.V. Ignatovskaya[2], V.I. Maksin[2], O.N. Iakubchak[2], D.O. Klymchuk[3]. **Stimuli-responsive properties of special micellar nanocarriers and their application for delivery of vitamin E and its analogues** *([1]Taras Shevchenko National University of Kiev, Ukraine, [2]National University of Life and Environmental Sciences of Ukraine, [3]M.G. Kholodny Institute of Botany, NAS of Ukraine, Kyiv).*

15:40 – 15:55 A.A. Yanovska[1,2], S.B. Bolshanina[1], A.S. Stanislavov[1,2], V.N. Kuznetsov[1,2], A.B. Mospan[1], V.Yu. Illiashenko[2], Yu.V. Rogulsky[2]. **Synthesis and characterization of Cu-loaded hydroxyapatite-alginate microspheres** *([1]Sumy State University, Ukraine, [2]Institute of Applied Physics, NAS of Ukraine, Sumy).*

15:55 – 16:10 M. Sęczkowska, A.W. Marczewski, A. Deryło-Marczewska, A. Chrzanowska. **Study of influence of process conditions on adsorption kinetics for 4-nitrophenol on active carbon** *([1]Faculty of Chemistry, Maria Curie-Skłodowska University, Lublin, Poland).*

16:10 – 16:30 coffee break

16:30 – 17:15 ***Poster session I (1-65)***

May 25, Thursday

Oral Session 4
Chair: ***PhD (Phys. & Math.) S. Snegir***

10:00 – 10:20 S.I. Pokutnyi. **New nanoheterostructures: artificial atoms and quasimolecules** *(Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv).*

10:20 – 10:40 O.Yu. Semchuk. **Features of absorption and emission of laser irradiation by free electrons in ferromagnetic semiconductors** *(Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv).*

10:40 – 10:55 **A. Ievtushenko**[1], P. Lytvyn[2], A. Korchovyi[2], V. Karpyna[1], O. Olifan[1], S. Korichev[1], S. Starik[3], S. Tkach[3], E. Kuzmenko[3], V. Baturin[4], O. Karpenko[4], G. Lashkarev[1]. **The structure, morphology and optical properties of nanostructured NiO thin films deposited by magnetron sputtering at diverse conditions** *([1]I. Frantsevich Institute for Problems of Material Science, NAS of Ukraine, [2]V. Lashkarev Institute of Semiconductor Physics, NAS of Ukraine, [3]V. Bakul Institute for Superhard Materials, NAS of Ukraine, Kyiv, [4]Institute of Applied Physics, NAS of Ukraine, Sumy).*

10:55 – 11:10 S.V. Dukarov, **S.I. Petrushenko**, V.N. Sukhov, O.I. Skryl. **Solubility in thin Cu-Pb and Cu-Bi films** *(V.N. Karazin Kharkiv National University, Ukraine).*

11:10 – 11:25 **S.I. Petrushenko**, S.V. Dukarov, V.N. Sukhov, O.O. Nevgasimov. **Thermal dispersion of polycrystalline Cu and Cu-Pb films** *(V.N. Karazin Kharkiv National University, Ukraine).*

11:25 – 11:45 coffee break

Oral Session 5
Chair: ***PhD (Chem.) O. Linnik***

11:45 – 12:05 **I.Yu. Zavaliy**[1], Yu.V. Verbovytskyy[1], A.R. Kytsya[2], P.Yu. Zavalij[3], P.Ya. Lyutyy[1]. **Influence of nano-additives on hydrogenation properties of R-Mg-Ni-based composites** *([1]Physico-Mechanical Institute, NAS of Ukraine, [2]Department of Physical Chemistry of Fossil Fuels InPOCC, NAS of Ukraine, Lviv, [3]Department of Chemistry and Biochemistry, University of Maryland, USA).*

12:05 – 12:20 **I.V. Levchenko**, V.M. Tomashyk, I.B. Stratiychuk, G.P. Malanych, A.A. Korchovyi, S.B. Kryvyi. **Features of the interaction between InAs, InSb, GaAs and GaSb and $(NH_4)_2Cr_2O_7-HBr-C_4H_6O_6$ mixtures** *(V. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine, Kyiv).*

12:20 – 12:35 **O.V. Sachuk**, V.A. Zazhigalov. **Physicochemical studies of mechanochemically modified CeO_2-MoO_3 system** *(Institute for Sorption and Problems of Endoecology, NAS of Ukraine, Kyiv).*

12:35 – 12:50 G.V. Lisachuk, **R.V. Krivobok**, E.V. Chefranov, O.M. Lapuzina, P.S. Korablova, I.G. Krasyuk. **The structure and phase composition of the radiotransparent ceramics** *(National Technical University «Kharkiv Polytechnic Institute», Ukraine).*

12:50 – 13:05 **V.V. Payentko**, E.M. Pakhlov, L.P. Golovkova, V.M. Gun’ko. **Mechanochemical preparation of powder composites with pollen and inorganic carriers** *(Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv).*

13:05 – 14:00 break

Oral Session 6
Chair: ***PhD (Chem.) T. Gromovoy***

14:00 – 14:20 S.S. Kotsyuda[1], P.V. Vakuliuk[1], I.M. Furtat[1], A.P. Lebed[1], O.O. Bilyayeva[2], **A.A. Golub**[1]. **Hybrid antibacterial nanocomposites based on silica** *([1]National University of Kyiv-Mohyla Academy, Faculty of Natural Sciences, [2]P.L. Shupik National Medical Academy of Postgraduate Education, Kyiv, Ukraine).*

14:20 – 14:40 **O.A. Viltsanyuk**[1], R.A. Lutkovskyy[2], N.M. Rezanova[3]. **Justification efficacy of nanocomposite mesh implants for treatment of abdominal hernias** *([1,2]Vinnitsa National Pirogov Memorial Medical University, Ukraine, [3]Kyiv National University of Technology and Design, Ukraine).*

14:40 – 15:00 **T.B. Zheltonozhskaya**[1], N.M. Permyakova[1], D.O. Klymchuk[2], L.R. Kunitskaya[1], V.I. Maksin[3], O.O. Kravchenko[3]. **Silver nanoparticle formation in micelles and micelle-like structures of heteropolymers** *([1]Taras Shevchenko National University of Kyiv, Ukraine, [2]M.G. Kholodny Institute of Botany, NAS of Ukraine, [3]National University of Life and Environmental Sciences of Ukraine, Kyiv).*

15:00 – 15:15 Iu.P. Mukha, **N.V. Vityuk**, A.M. Eremenko. **Mono- and bimetallic nanoparticles of silver and gold for cancer treatment** *(Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv).*

15:15 – 15:30 **O.O. Kravchenko**[1], V.I. Maksin[1], T.B. Zheltonozhskaya[2], N.M. Permyakova[2]. **Biological activity and toxicity assessment of polymer/silver composition** *([1]National University of Life and Environmental Sciences of Ukraine, Kyiv, [2]Taras Shevchenko National University of Kyiv, Ukraine).*

15:30 – 15:45 **G.A. Dolynskyi**, O.M. Lavrynenko, Yu.S. Shchukin. **Enzyme mimetic activity of nanosized cerium dioxide following different surface modification** *(Institute for Problems in Material Science, NAS of Ukraine, Kyiv).*

15:45 – 16:00 **A. Chrzanowska**, A. Derylo-Marczewska, A.W. Marczewski, M. Sęczkowska. **Structural and surface properties of biocomposite protein/mesoporous silica** *(Faculty of Chemistry, Maria Curie-Sklodowska University, Lublin, Poland).*

16:00 – 16:15 **M. Zienkiewicz-Strzalka**, A. Derylo-Marczewska, M. Blachnio. **Silver nanoparticles in composite systems** *(Faculty of Chemistry, Maria Curie-Sklodowska University, Lublin, Poland).*

16:15 – 16:35 coffee break

16:35 – 17:15 ***Poster session II (66-127)***

17:15 Conference Closing

Poster presentations

1. Theory of chemical structure and reactivity of solid surface

1. **E.M. Demianenko**[1], O.S. Kukolevska[2], A.G. Grebenyuk[1], I.I. Gerashchenko[1]. **Simulation of adsorption complexes of 2-hydroxyethyl methacrylate on silica surface** *([1]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv, [2]Vinnytsia National Pirogov memorial Medical University, Ukraine).*
2. **R. Meshkini Far**, A. Dyachenko, O. Bieda, E. Ischenko. **Surface composition effect of Ni-Fe catalysts in the reaction of CO_2 methanation** *(Faculty of Chemistry, Taras Shevchenko National University of Kyiv, Ukraine).*
3. **A.A. Kravchenko**, E.M. Demianenko, O.V. Filonenko, A.G. Grebenyuk, V.V. Lobanov, M.I. Terets. **A quantum chemical analysis of dependence of the protolytic properties of polysilicate acids on the composition and spatial structures of their molecules** *(Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv).*
4. **D.B. Nasiedkin**, Yu.V. Plyuto, A.G. Grebenyuk. **DFT study on reactivity of graphite carbon atoms in basal-plane positions** *(Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv).*
5. **A.M. Puziy**[1], O.I. Poddubnaya[1], T.Yu. Gromovoy[2]. **LDI-ToF investigation of carbon catalyst's surface** *([1]Institute for Sorption and Problems of Endoecology, NAS of Ukraine, [2]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv).*
6. **O. Smirnova**, A. Grebenyuk, V. Lobanov. **Theoretical investigation of pollutant species adsorption on oxygen vacancies or pure and nitrogen-doped titania** *(Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv).*
7. **M.I. Terebinska**, O.I. Tkachuk, V.V. Lobanov. **Effect of SiO_2 dielectric film on the properties of Ge quantum dots** *(Chuiko Institute of Surface Chemistry of NAS of Ukraine, Kyiv).*
8. **A.V. Vakaliuk**, L.M. Grishchenko, T.M. Bezugla. **Acid-base catalysts based on carbon fibers** *(Taras Shevchenko National University of Kyiv, Ukraine).*

2. Physical chemistry of surface phenomena

9. **O. Ananina**[1], N. Lvova[2]. **Modeling of fluorine atoms interaction with the fluorinated diamond surface** *([1]Zaporizhzhya National University, Physical Faculty, Ukraine, [2]Technological Institute for Superhard and Novel Carbon Materials, Troitsk, Russia).*
10. **O.E. Bashchak**[1], I.A. Kovalchuk[1], V.Yu. Tobilko[2], B.Yu. Kornilovych[1,2]. **Pillared layer silicates with iron nanoparticles for heavy metals removal from aqueous solution** *([1]Institute for Sorption and Problems of Endoecology, NAS of Ukraine, Kyiv, [2]Igor Sikorsky Kyiv Polytechnic Institute, Ukraine).*
11. **M. Blachnio**, M. Zienkiewicz-Strzałka, A. Derylo-Marczewska, A.W. Marczewski, Sz. Winter. **Studies of dyes adsorption equilibria and kinetics on activated carbons** *(Faculty of Chemistry, Maria Curie-Sklodowska University, Lublin, Poland).*

12. **M. Blachnio**, M. Zienkiewicz-Strzałka, A. Derylo-Marczewska, A.W. Marczewski. **Influence of structural and surface properties of activated carbon on adsorption of pesticides – adsorption equilibrium and kinetics** *(Faculty of Chemistry, Maria Curie-Sklodowska University, Lublin, Poland).*
13. **Yu. Bolbukh**[1], P. Klonos[2], V. Tertykh[1], P. Pissis[2]. **Polyvinylidene fluoride films with bifunctional silica nanofillers** *([1]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv, [2]National Technical University of Athens, Physics Department, Greece).*
14. **A. Chrzanowska**, A. Derylo-Marczewska, M. Sęczkowska. **UV-Vis DRS and ATR-FTIR spectroscopic studies of porous MCF silica surface with adsorbed lysozyme** *(Faculty of Chemistry, Maria Curie-Sklodowska University, Lublin, Poland).*
15. **A. Derylo-Marczewska**[1], M. Blachnio[1], A.W. Marczewski[1], T.M. Budnyak[2], V.A. Tertykh[2]. **Hybrid composites and their application for removal of sulfonated azo dyes from aqueous solutions** *([1]Faculty of Chemistry, Maria Curie-Sklodowska University, Lublin, Poland, [2]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv).*
16. **Ye.M. Fadieiev**, S.S. Smola, N.V. Rusakova. **Immobilization of luminescent Eu(III) *β*-diketonato-1,10-phenanthroline complexes on aerosils** *(A.V. Bogatsky Physico-Chemical Institute, NAS of Ukraine, Odessa).*
17. **T.V. Fesenko**, O.A. Kazakova, I.V. Laguta, O.N. Stavinskaya. **Ionization of flavonols in mass spectrometric experiment** *(Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv).*
18. **Yu.S. Fetisova**[1], V.V. Sliesarenko[2], O.A. Dudarko[2], Yu.L. Zub[2] **Adsorption of lead(II) and cadmium(II) ions by mesoporous silica functionalized with diethylphosphatoethyltriethoxysilane via direct template method** *([1]National University of "Kyiv-Mohyla Academy", Ukraine, [2]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv).*
19. **V. Galysh**[1,2], M. Kartel[1], W. Janusz[3], E. Skwarek[3]. **Strontium ions sorption on composite sorbent based on lignocellulose and hydrated antimony pentoxide** *([1]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv, [2]National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", Ukraine, [3]Department of Radiochemistry and Colloid Chemistry, Maria Curie-Sklodowska University, Lublin, Poland).*
20. **O.V. Goncharuk**[1], A.P. Ugnivenko[2], K. Terpilowski[3], E. Skwarek[3], V.M. Gun'ko[1]. **Effect of ethonium adsorption on structure formation in nanosilica dispersions** *([1]Chuiko Institute of Surface Chemistry, NAS of Ukraine, [2]Department for Biotechnical Problems of Diagnostic, IPCC, NAS of Ukraine, Kyiv, [3]Faculty of Chemistry, Maria Curie-Skłodowska University, Lublin, Poland).*
21. **A.M. Kostruba**[1], B.I. Rachiy[2], R.Y. Musiy[3]. **New ellipsometric technique for characterization of ultrathin thermo-responsive coatings in liquid ambient** *([1]Lviv University of Commerce and Economic, [2]Vasyl Stefanyk Precarpathian National University, Ivano-Frankivsk, Ukraine, [3]Department of Physical Chemistry of Fossil Fuels InPOCC, NAS of Ukraine, Lviv).*
22. **T. Kulik**[1], B. Palianytsia[1], K. Kulyk[2], M. Larsson[2], M. Kartel[1]. **The surface complexes of carboxylic acids and their thermal transformations into important "green" chemicals** *([1]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv, [2]Stockholm University, AlbaNova University Center, Department of Physics, Sweden).*

23. **T.N. Lygovitskaya**[1], S.S. Naboichenko[2]. **Intermolecular interactions of like-charged oligomeric electrolytes and surfactants in aqueous media** *([1]Saratov National Research University named after N.G. Chernyshevsky, [2]Ural Federal University named after the first President of Russia B.N. Yeltsin, Ekaterinburg, Russia).*
24. **F.D. Manilevich**, L.F. Kozin, A.I. Lisogor, A.V. Kutsyi. **Regularities of hydrogen evolution from water at modified tungsten carbide based cathodes** *(V.I. Vernadsky Institute of General and Inorganic Chemistry, NAS of Ukraine, Kyiv).*
25. **A.W. Marczewski**, M. Sęczkowska, A. Deryło-Marczewska. **Study of dyes adsorption on carbon materials in the multicomponent system** *(Faculty of Chemistry, Maria Curie-Skłodowska University, Lublin, Poland).*
26. **O.O. Ovcharenko**, N.D. Sakhnenko, M.V. Ved'. **Corrosion resistance of nanocomposite electrochemical coatings** $Ni\text{-}Al_2O_3$ *(National Technical University "Kharkiv Polytechnic Institute", Ukraine).*
27. **O.A. Ozerov**[1], V.I. Kovalchuk[2], E.K. Zholkovskiy[3]. **Broadening of analyte bands in electroosmotic flow through microchannels with different zeta potentials of walls. Pre-Taylor asymptotic regime** *([1]F.D. Ovcharenko Institute of Biocolloidal Chemistry, NAS of Ukraine, Kyiv).*
28. **V.A. Petrova**, V.V. Garbuz. **Sorption-desorption of nitrogen on the surface turbostratic graphene-like boron nitride** *(Institute for Problems of Materials Science, NAS of Ukraine, Department for Methods of Analyses of the Inorganic Materials, Kyiv).*
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3. Chemistry, physics and technology of nanomaterials

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50. **N. Dolaberidze**, V. Tsitsishvili, M. Nijaradze, N. Mirdzveli. **Preparation of fine dispersed sodalite by hydrothermal modification of natural clinoptilolite** *(Petre Melikishvili Institute of Physical and Organic Chemistry; Ivane Javakhishvili Tbilisi State University, Georgia).*
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55. **V.A. Gigiberiya**. **Self-organization of carbon nanotubes in evaporating droplets of toluene and isopropanol suspensions with presence of Triton X-165** *(F.D. Ovcharenko Institute of Biocolloidal Chemistry, NAS of Ukraine, Kyiv).*
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62. **O.O. Havryliuk**, O.Yu. Semchuk. **Optimization of size of periodic structures for solar cells** *(Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv)*.

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92. **A.M. Sklyar**[2], O.V. Kalinkevich[1], V.D. Chivanov[1], S.V. Novikov[1], A.G. Ryabyshev[1], A.N. Kalinkevich[1], S.N. Danilchenko[1]. **Characterization of chitosan iodide by temperature-programmed desorption mass spectrometry method** *([1]Institute of Applied Physics, NAS of Ukraine, Sumy, [2]Sumy State Pedagogical University, Ukraine).*
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95. **S.S. Smola**, Ye.M. Fadieiev, N.V. Rusakova. **Synthesis and luminescent properties of hybrid SiO_2 and SiO_2/TiO_2 materials doped with Ln(III) aminopolycarboxylates** *(A.V. Bogatsky Physico-Chemical Institute, NAS of Ukraine, Odessa).*
96. **D.L. Starokadomsky**. **Epoxy composites filled with initial and water-hardened inorganic binders (gypsum, cement, chalk)** *(Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv).*
97. **G.M. Starukh**[1], V.L. Budzinska[2]. **Application of organo/layered double hydroxides for the preparation of polyurethane nanocomposites** *([1]Chuiko Institute of Surface Chemistry, NAS of Ukraine, [2]Institute of Macromolecular Chemistry, NAS of Ukraine, Kyiv).*

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99. **V. Sydorchuk**, S. Khalameida, O. Poddubnaya, A. Puziy. **Cu- and Co-containing active carbons as photocatalysts for rhodamine B degradation** *(Institute for Sorption and Problems of Endoecology, NAS of Ukraine, Kyiv).*
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4. Medical, biological and biochemical aspects of research of highly disperse materials

104. **M.V. Abramov**[1], A.P. Kusyak[2], O.M. Kaminskiy[2], S.P. Turanska[1], A.L. Petranovska[1], N.V. Kusyak[2], P.P. Gorbyk[1]. **Magnetosensitive nanocomposites based on cisplatin and doxorubicin for application in oncology: control of size parameters and bioactivity** *([1]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv, [2]Ivan Franko Zhytomyr State University, Ukraine).*
105. **L.S. Andriyko**[1], V.M. Gun’ko[1], V.V. Turov[1], T.V. Krupska[1], A.I. Marynin[2], A.I. Ukrainets[2]. **Interaction of doxorubicin with human serum albumin in the nanosilica presence** *([1]Chuiko Institute of Surface Chemistry, NAS of Ukraine, [2]National University of Food Technology, Kyiv, Ukraine).*
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Synthesis and magnetic properties of yttrium iron garnet nanoparticles

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Since their discovery in 1956 by Bertaut and Forrat [1], Yttrium Iron Garnet ($Y_3Fe_5O_{12}$, YIG) have attracted attention due to their interesting properties, as low dielectric loss, narrow resonance linewidth in microwave region and good saturated magnetization value, and as an important material in optical communication and magneto-optical devices [2].

Single-phase YIG nanocrystals have been synthesized via a chemical coprecipitation process. The nanocrystals calcined at 910, 960, 980 ^{o}C belonged to a garnet phase and were of 30, 36 and 40 nm in average size, respectively.

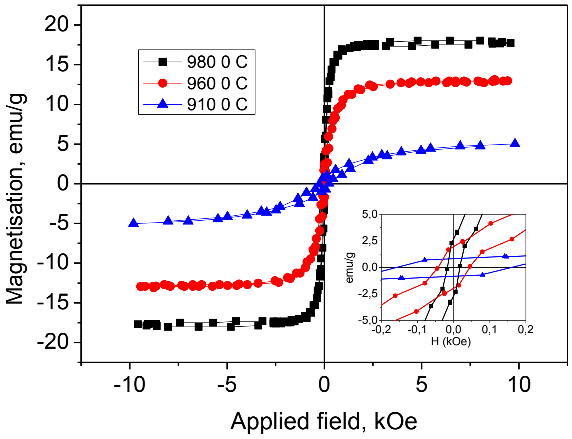

Fig. Hysteresis loops recorded at the temperature of 300 K for the samples sintered at three different temperatures. The inset shows the initial area of hysteresis loops

The room temperature saturation magnetization of the samples after calcinations at various temperatures showed a nonlinear increase from 5.0 to 18.4 emu/g.

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Magnetosensitive nanocomposites based on cisplatin and doxorubicin for application in oncology: control of size parameters and bioactivity

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Investigations are directed onto development of the concept of creation of magnetosensitive nanocomposites with multilevel hierarchical nanoarchitecture and functions of biomedical nanorobots [1].

We synthesized nanosized magnetite in single-domain state and magnetosensitive nanocomposites (NC) based on that with various chemical nature of surface (Fe_3O_4/dimercaptosuccinic acid, Fe_3O_4/3-aminopropylsiloxane, Fe_3O_4/polyacrylamide, Fe_3O_4/hydroxyapatite (HA), Fe_3O_4/SiO_2, Fe_3O_4/TiO_2, Fe_3O_4/Al_2O_3). Isotherms and adsorption kinetics of cisplatin were studied depending on chemical nature of the surface of nanostructures. Adsorption of doxorubicin (DOX) onto the surface of Fe_3O_4/HA NC from solution in physiological liquid was studied. Magnetic fluids containing Fe_3O_4/HA/DOX NC were produced and investigated. Using an ensemble of Fe_3O_4 carriers as a superparamagnetic probe, the Langeven paramagnetism theory, we appreciated size parameters of their shell, which was confirmed by independent measurements of specific surface area of the nanostructures and kinetic stability of the corresponding magnetic fluids. Cytotoxic and antiproliferative activity of the magnetosensitive nanocomposites containing cisplatin or doxorubicin were studied with respect to yeast cells *Saccharomyces cerevisiae*. Mechanism of action of nanocomposites was determined to coincide with typical influence of the cytostatic preparation, which permitted to work fairly effective, reliable, safe and relatively inexpensive technique of before-clinical control of cytotoxic activity of nanocomposites.

The results obtained may be used in development of new forms of magnetocarried medical remedies for targeted delivery and adsorbents based on nanocomposites of superparamagnetic core-shell type with multilevel nanoarchitecture, and for determination, control and optimization of their parameters.

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Modeling of fluorine atoms interaction with the fluorinated diamond surface

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Diamond is a material comprising a number of unique properties. Various applications of synthetic diamond often require a considerable effort in preparing a perfect surface. Another important target is to provide a surface relief structure with desired geometrical characteristics. A promising method of preparing a diamond surface is its reactive ion plasma etching (RIE) in gas mixtures containing fluorine atoms [1]. This method involves an interaction of the active particles with the surface, and this type of impact is inevitably accompanied by a significant number of defects. However, the mechanisms of chemical interaction between F atoms and F-containing molecules and fragments with the defects on the diamond surface remain underinvestigated.

In this paper, we present the results of quantum-chemical calculations of the interaction of fluorine atoms F, as well as CF_2 and CF_3 particles, with the ordered and defective C(100)-(2×1) diamond surfaces. We discuss the possible degree of fluorine coating for an ordered C(100)-(2×1) surface. We applied the approach developed earlier [2].

We used the C_mH_k clusters as model objects to simulate the C(100)-2×1 diamond surfaces. We calculated the cluster energy, bond orders, atomic orbitals population, molecular and localized orbitals. We provide a comparison between the processes of F atoms interaction with an ordered and defect cluster surface. We investigated the interactions of fluorine atoms and F-containing fragments with different types of surface defects. Preliminary calculations indicate a possibility of smoothing out the diamond surface when the CF_2 radicals are adsorbed from the gas mixture. It may be assumed that in the reactive fluorine atmosphere a lot of vacancies are formed, the occurrence of which initiates the further formation of linear defects.

The results can be used to analyze the physical and chemical processes on the diamond surface during RIE using halogen-based plasma.

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The interaction of doxorubicin with human serum albumin in the nanosilica presence

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Although doxorubicin (DOX) has been used as an anti-cancer drug during a long period, it remains a popular medicine for chemotherapeutical applications to treat various cancers. It is frequently used in conjugates with such compounds as human serum albumin (HSA) as a transport protein. The albumin molecules playing a typical role of a drug carrier in the delivery system promote fast penetration of the DOX molecules into cancer cells. The drug delivery system based on HSA is a natural one and, therefore, could be more preferable.

The aim of this work is a study of interactions of DOX with HSA molecules and binding HSA-DOX complex with a nanosilica surface using laser correlation spectroscopy (LCS).

The solution of initial DOX (C_{DOX}=18.92·10^{-5} mol/l), HSA-DOX complex (C_{Protein} = 1.54·10^{-4} mol/l), and its binding with the nanosilica surface were studied in aqueous medium. It was found that the diameter of particles in the solution of initial DOX is 450 and 950 nm. The interaction of DOX molecules with HSA molecules leads to binding and formation of HSA-DOX complex having the diameter of 5 nm (corresponding to the size of the protein globules). Addition the aqueous suspension of nanosilica (C = 5 wt. %, sonicated for 5 min) to HSA-DOX complex results in the creation of structures with size of 100 nm.

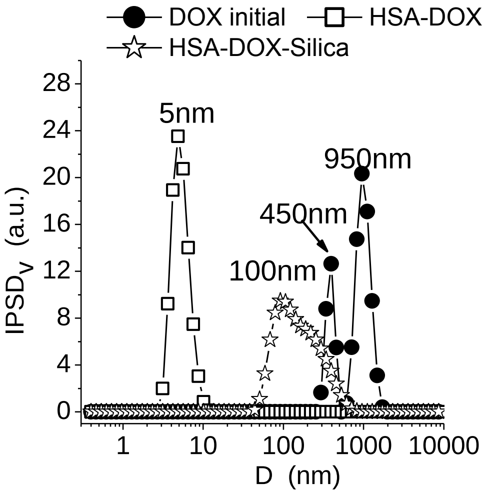

Fig. Particle size distribution with respect to the volume in the solution of initial DOX, HSA-DOX complex and HSA-DOX-silica in aqueous medium

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Influence of the platinum additives on sensitivity to H_2 adsorption of semiconductor hydrogen sensors based on nanosized tin dioxide

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Nowadays hydrogen is the most clean and ecological energy source and therefore it is the most promising area of the energy industry. Development of devices on the base of adsorption-semiconductor sensors for H_2 detection in air is actual and important issue. It is known that catalytic active additives are introduced in the gas-sensitive sensor layers to increase responses of the sensors. We chose to study the parameters of the sensors based on Pt/SnO_2 nanomaterial since the platinum is active catalyst for hydrogen oxidation.

A ratio of the electric resistance in air (R_0) of the sensor to the electric sensor resistance in a hydrogen–air mixture containing 40 ppm H_2 (R_g) was taken as a measure of sensitivity of the sensor ($\gamma = R_0/R_g$). The sensors with different Pt contents were created on the base of the nanosized tin dioxide by its impregnation with H_2PtCl_6 solutions of different concentrations (0.21×10^{-2} - 35×10^{-2} M). An extremal dependence of the electrical resistance in air on concentration of H_2PtCl_6 solution was established (Fig. 1). It was found, when the temperature is increased the maximums of the sensor responses are shifted to the region of lower concentration of the H_2PtCl_6 solutions (Fig. 2). It was established that catalytic activity of Pt/SnO_2 nanomaterial in a great extent influences on the sensor response value. That is why catalytic reaction of hydrogen oxidation running on the sensor surface is crucial in the formation of the sensor response.

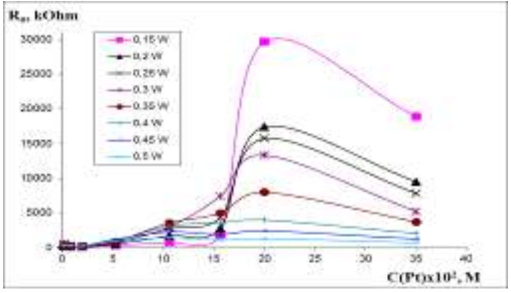

Fig. 1. Dependence of the sensor electric resistance in air on concentration of H_2PtCl_6 solution at different heater power consumption of the sensor

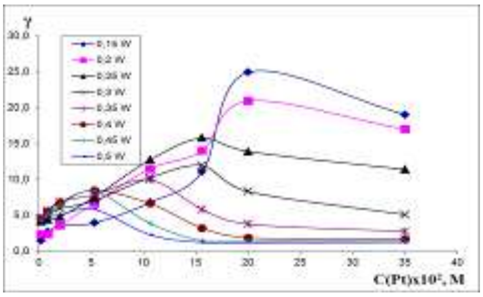

Fig. 2. Dependence of the sensor response to 40 ppm H_2 on concentration of H_2PtCl_6 solution at different heater power consumption of the sensor

Investigation of the endogenous metabolism of yeast cells *Saccharomyces cerevisiae* in an aqueous medium in the presence of graphene nanoplates

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Carbon-based nanoparticles (fullerenes and their derivatives, graphene and carbon nanotubes) are a broad class of materials that have potential biomedical applications. Investigations of the influence of these materials on microorganisms also contribute to understanding the safe use of graphene materials in various fields of scientific and technical applications, including medical applications. There are very contradictory data on the effect of graphene nanoplates on the intensity of life of unicellular organisms.

The aim of the work is to study the processes of vital activity of yeast *Saccharomyces cerevisiae* under conditions of endogenous metabolism in the presence of graphene nanoplates.

The dehydrated industrial yeast *Saccharomyces cerevisiae* produced by Saf-Levur was used as a biological object. Studies of endogenous metabolism in the anaerobic conditions of cells were carried out in the tap water using a differential microcalorimeter (DMC) under isothermal conditions (295 ± 0.5 K). The sensitivity of the DMC on the heat flux was 10^{-6} W. For the study, graphene obtained by electrochemical dispersion of graphite electrodes in an alkaline electrolyte (KOH) of low concentration with a current transmission to 60 mA/cm^2 was used. The studies were carried out in the concentration range 0.35 – 3%.

An analysis of the experimental values of the thermal effect in endogenous metabolism, which characterizes the enzymatic activity of yeast cells depending on the content of graphene nanoplates, indicates a very complex character of the change in yeast cell activity in the presence of graphene nanoparticles. The concentration curve characterizing the enzymatic activity of cells has a maximum of about 0.75% mass., which reflects the achievement of maximum activation of the vital activity of yeast. It is probably the result of stress response in yeast on alarm stage and is explained the phenomenon hormezys.

Further increasing concentrations of graphene nanoplates to 3% mass. leads to the inhibition in cells of fermentation activity, but with this, time process of fermentation increases.

Pillared layer silicates with iron nanoparticles for heavy metals removal from aqueous solution

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Nanomaterials based on clay minerals have wide prospects of applying for the environmental protection. One of the possible approaches improving selectivity clay sorbents for their application for extraction of heavy metals and radionuclides from aquatic environment is applying of nanocomposites based on nanoiron. But the disadvantages of such systems are the essential tendency of particles to aggregation and a high speed of oxidation. One of the ways of slowing down these processes is immobilization of particles of nanoiron on the surface of the dispersed inorganic matrix – montmorillonite particles. In other side montmorillonite can be easily modified by intercalating inorganic cations and the resulting products are more efficient adsorbents for removing the anions by clay minerals than the original one, due to the formation of regular porous structures, called pillared clays.

The purpose of this study was to investigate novel composite of Al-, Fe-pillared montmorillonite with nanoiron for the removal of heavy metals from contaminated water.

As a result of conducted studies, iron-containing materials were synthesized on the basis of pillared montmorillonite because it is known that the formation of regular porous structures allows influencing the course of processes on it. Al and Fe polynuclear hydroxocomplexes as pillared agents and sodium borohydride ($NaBH_4$) as reducing agent were used in the experiments. It was proved that pillared montmorillonite contributes to the formation of more dispersed particles of nanoiron.

The extraction of uranium from solutions can occur by two parallel mechanisms: sorption and reduction. With the first one, the anionic forms of uranium are sorbed by active sites of hydroxide film formed on the surface of iron nanoparticles due to their partial oxidation (so-called “core-shell” structure). With the second one, hexavalent uranium is reduced by nanodispersed zero-valent iron to the lower valent state.

It was established that the synthesized nanocomposite extracts up to 0.1 g/g of Fe ions, Co(II) and U(VI), which is much more efficient in comparison with the iron-containing sorbents that do not contain pillared montmorillonite.

Functionalization of magnetite nanoparticles with mercaptopropyl groups using 1,2-*bis*(triethoxysilyl)ethane

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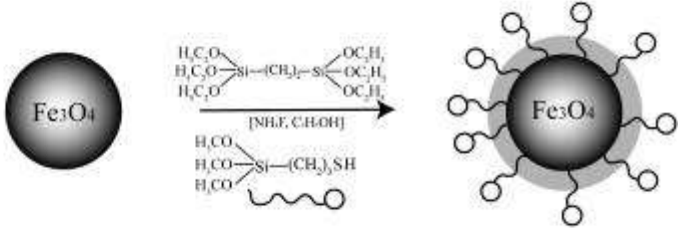
Composite materials based on magnetite nanoparticles functionalized with mercaptopropyl groups have been widely used as adsorbents for the removal of heavy and precious metal ions from water solutions. The presence of magnetic core makes it possible to remove the sorbent from working solutions after sorption quickly and effectively, compared with conventional silica gel sorbents.

The aim of this work was to functionalize the nanoparticles of magnetite with 3-mercaptopropyl groups via sol-gel method, using 1,2-*bis*(triethoxysilyl)ethane as a structuring agent.



Through the organic bridge, this *bis*-silane provides additional impact on the nature of the surface of the obtained particles by reducing the steric difficulties and improving access of target ions to the functional groups by increasing the distance between them.

Particle morphology and composition of the surface layer were analyzed by SEM and IR spectroscopy. The resulting materials are magnetically controllable particles with the surface siloxane bonds, hydrocarbon bridges and mercaptopropyl groups. The study of the sorption properties shows the possibility of using such materials as sorbents of heavy metal ions. Our studies also indicate the possibility of modifying nanoparticles with other functional groups.

Acknowledgements
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Studies of dyes adsorption equilibria and kinetics on activated carbons

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Dyes due to their hazardous effects on organisms, even at very low concentrations are undesirable compounds in waters. They are widely employed in the textile, pharmaceutical, food, cosmetics, plastics, photographic and paper industries. It is estimated that more than 10000 various dyes and pigments are used industrially and over $7 \cdot 10^5$ tons of the synthetic dyes are annually produced worldwide, with about 10–15% of them lost to effluents during manufacturing process. In the textile industry alone, up to 200000 tons (per year) of dyes is released in the environment due to inefficiency of the manufacturing processes.

Typical dyes are stable, resistant to light, heat and biodegradation [1] limiting the efficiency of conventional water treatment techniques [2]. As alternative method, introduction of adsorption process in the treatment can be used due to simple design, efficiency, low initial cost, ease of operation and flexibility – typically with microporous activated carbons as adsorbents. However, the molecular dimensions of most dyes are close to upper limit of micropore size, making mesoporous carbons more suitable as adsorbents.

In this work the process of dye adsorption is studied on the chosen commercial microporous and a few mesoporous carbons of divergent porosity synthesized by the method of impregnation of mesoporous silicas obtained by applying the Pluronic copolymers as pore creating agents. Both adsorption isotherms and kinetic curves from aqueous solutions of dyes on activated carbons with differentiated porosity were measured by means of UV/Vis spectrophotometer. The experimental isotherms were interpreted on the basis of the Generalized Langmuir (GL) equation while kinetics by applying various equations: first order equation (FOE), second order equation (SOE), mixed 1.2-order equation (MOE), multi-exponential equation. The dependences between the properties of adsorbates and adsorbents, and adsorption rate were analyzed.

Acknowledgements

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Influence of structural and surface properties of activated carbon on adsorption of pesticides – adsorption equilibrium and kinetics

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A major problem concerning the environment protection is pollution of waters and wastewaters with pesticides. Although the pesticides production adapts to more restrictive regulations concerning their registration and outlines determining the set on the market, these substances are still a threat to the living organisms because of toxicity, persistence, mobility and bioaccumulation [1]. Among the most used pesticides in the agriculture should be mentioned compounds like: 4-chlorophenoxyacetic acid (4-CPA), 2.4-dichlorophenoxyacetic acid (2.4-D) and 4-chloro-2-methylphenoxyacetic acid (MCPA). Due to low adsorption coefficients and high solubility, they have been frequently detected in waters [2]. As neutral for the environment, the adsorption methods involving a purification of waters and wastewaters using activated carbon as an adsorbent have been widely applied. Despite satisfactory adsorption efficiency of carbon adsorbents towards organic pollutants, the literature is abundant with research attempting to improve such processes, including the influence of adsorbent, adsorbate, solution properties and conditions of adsorption process.

The aim of the present paper is to estimate dependence between the surface chemistry of oxidized and unmodified activated carbons and adsorption of aromatic pesticides from dilute aqueous solutions. Both adsorption isotherms and concentration profiles of 4-CPA, 2.4-D and MCPA on activated carbons with differentiated surface chemistry were measured. The textural and chemical characteristics of the carbons surface and evaluation of their adsorption capacity for the pesticides were carried out. The experimental isotherms were interpreted on the basis of the Generalized Langmuir (GL) equation. The kinetic data were analyzed applying various theoretical models and equations. The obtained data were discussed in order to find the correlations between changes in the chemical properties of the carbons surface and parameters characterizing adsorption equilibria and kinetics.

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Synthesis and adsorption characteristics of Co/C composites produced from sunflower seed shells

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Sunflower is an important agricultural crop in Ukraine. 13.3 million tons of a sunflower seed were harvested in 2016. Sunflower seed shells (SSS) can be a valuable raw material to obtain new carbon-inorganic composites. Thus, magnetically sensitive Co-doped carbon adsorbents on the base of cheap sunflower shells had been study in this work.

SSS were impregnated by salt of $CoCl_2{\cdot}6H_2O$ in different solutions. Water, NH_4OH or isopropanol alcohol were used as the solvents (labeled as 2Co/C, 3Co/C, 4Co/C, respectively). Then the samples were dried at 150 °C under air atmosphere and carbonized at 800 °C in flow of argon. This approach leads to formation of a phase of metallic cobalt in porous black carbons. XRD, low-temperature N_2 adsorption-desorption, thermogravimetry and adsorption of methylene blue were used to investigate new composites.

The cubic and hexagonal crystalline forms of cobalt were detected in all synthesized samples. All the composites were magnetically sensitive. The structural characteristics of the samples were obtained from adsorption data (Table). The pore size distribution shows the microporous structure of all composites. The maximum adsorption of methylene blue was 120, 150 and 140 mg per g of composite for 2Co/C, 3Co/C and 4Co/C, respectively.

Samples	2Co/C	3Co/C	4Co/C
S_{BET}, m^2/g	383	371	387
V_{pore}, cm^3/g	0.184	0.171	0.181

Thus, magnetically sensitive nanocomposites of metal cobalt@black carbon were successfully obtained by carbonize of the sunflower shells with cobalt chloride.

Acknowledgements
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Synthesis and algicidal effect of disperse silica modified with Cu and Zn oxides compounds

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Harmful algal blooms in the pools and different tanks may be prevented by using algicidal materials. Algicidal effect of new silica nanocomposites, containing surface oxide species of copper and zinc had been study in this report.

Nanocomposites were obtained via modification of precipitated silica with surface area of 130 m^2/g by ammonia complexes of copper and zinc with subsequent thermal treatment at 200 °C and formation of nanooxide species of Cu and Zn on the silica surface. Content of the metals in the nanocomposites was 0.2, 0.5 and 1.0 mmol/g SiO_2 (labeled as 02, 05 and 10, respectively). The copper and zinc content in the binary systems corresponded to a molar ratio of 1:1. Thermogravimetry, UV-Vis spectroscopy, chromatography and XRD methods were used to characterize nanocomposites.

Algicidal activity against green algae was determined by the holes method in Petri dishes using agar medium for algae at 26 ± 1 °C, and efficacy was assessed by the measuring the diameter of the growth inhibition zone of cultures and expressed in mm as the average for three experiments (table).

Samples	Diameter of growth inhibition zone of algae, mm									
	Chlorela vulgaris Strain number							*Chlorela kessleri* Strain number		
	190	191	192	193	326	327	500	200	201	205
02 Cu	12	12	12	12	13	12	14	-	11	12
05 Cu	27	25	25	20	23	22	21	23	20	26
10 Cu	16	16	17	16	16	14	15	15	14	17
02 Zn	0	0	0	0	0	0	0	0	0	0
05 Zn	0	0	0	0	0	0	0	0	0	0
10 Zn	14	12	14	11	11	12	16	11	11	13
02 CuZn	0	0	0	0	0	0	0	0	0	0
05 CuZn	12	14	17	17	14	11	13	13	12	14
10 CuZn	28	26	25	28	24	26	24	23	20	25

Thus, the highest algicidal effect is observed in the samples of 05 Cu (0.5 mmol Cu/g SiO_2) and 10 CuZn (Cu 0.5 mmol/g and Zn 0.5 mmol/g SiO_2).

Polyvinylidene fluoride films with bifunctional silica nanofillers

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Four different crystalline phases can be detected for polyvinylidene fluoride (PVDF). These phases have capable of mutual transitions under the action of mechanical, electrical, thermal and radiation affect, as well as by precipitation in some types of solvents. The β-crystalline phase, which is responsible for the nature of the piezo and pyroelectrical effects in PVDF material, has the greatest scientific and technical interest. This phase is formed during drawing orientation of films or at the recrystallization from solutions of some solvents. Also, β-crystalline phase formation is affected at introduction of the modifying additives into the polymer chain. The aim of this work was to study possible changes in the structure of the crystalline phase of PVDF in the presence of silica nanofillers with different surface functionality.

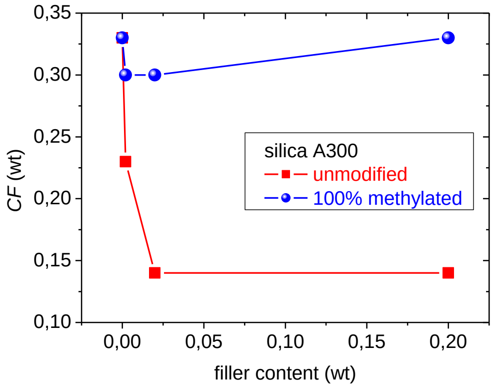

Fig. Contents of the crystalline phase (CF) in PVDF films with unmodified (A300) and methylated fumed silicas at the different filling degree

PVDF films were prepared by polymer dissolving in dimethylsulfoxide at heating to 60 °C. The resulting solution was mixed with the filler using ultrasonication. Fumed silicas with different functional groups and the degree of surface modification were used for filling. Separated from the plate films were investigated using DSC in a temperature range of -80 to 150 °C. The figure shows data for films with pristine and methylated silica.

The results indicate a decrease in the crystallinity degree when the filler is used. The effect is less significant for methylated silica. At the same time, the structure of the crystalline phase was more uniform in comparison with the unfilled polymer, which can be applied later to produce oriented films.

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The number of electronic states at the Fermi level as a criterion of impact sensitivity

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Quantum-chemical calculations are the most popular methods for evaluation of impact sensitivity [1]. Earlier, the effect of band gap values on impact sensitivity was specified for metal azides listed in Table 1 [2]. The revealed dependence, however, has only qualitative character. On the other hand, this dependence is very important since it specifies the fundamental role of the electron transition energies from valence to conduction bands in governing impact sensitivity. It is obvious that the number of states at the Fermi level (N_{states}) is crucial for determination of the electron transition probability. The conduction bands have antibonding character and when these are occupied, the structure starts to decompose.

In order to support this hypothesis we have calculated band structures and partial density of states (PDOS) for the metal azides (Table). The plot of integrated DOS for CuN_3 is illustrated in Fig., *a*. Remarkably, N_{states} correlates well with the impact sensitivity (*IS*). The obtained plot is illustrated in Fig., *b* and the numerical values of *IS*, which are based on the obtained regression equation, are listed in Table. Experiments revealed that alkaline metal azides are insensitive to impact [2]. Meanwhile, the correlation predicts that KN_3 is only slightly less sensitive than TlN_3 (18.87 *vs*. 16.84 kg m cm^{-2}). Thus, the other factors should exist to affect impact sensitivity. By accounting these factors, one can safely distinguish sensitive and insensitive materials. Probably, these factors are the following: band gap, crystal morphology and bulk modulus.

Table. The values of N_{states} at the Fermi level and the corresponding impact sensitivities (kg m cm^{-2})

Parameter	LiN_3	NaN_3	KN_3	CuN_3	TlN_3	AgN_3
N_{states}	16	25	49	104	56	69
IS_{exper}	none	none	none	2.66	16.18	13.97
IS_{theor}	28.45	25.84	18.87	2.90	16.84	13.07

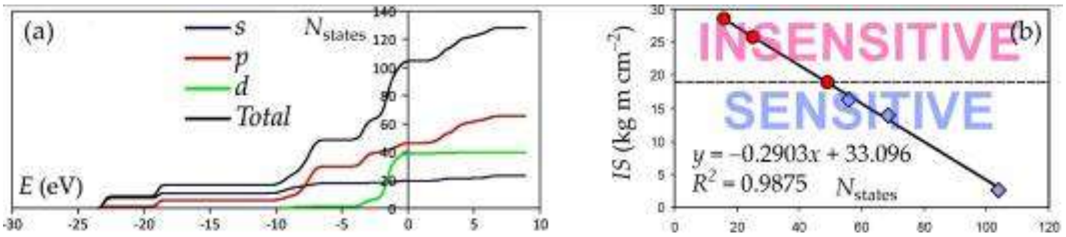

Fig. Integrated density of states for CuN_3 (*a*) and plot of impact sensitivity against N_{states} (*b*)

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Photocatalytic properties of S/C/TiO_2 nanocomposites

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Nowadays researchers pay much attention to investigations of such disperse nanomeasured titanium-dioxide-based composite materials that may be applied to ecological photocatalysis for industrial waste-water purification from various pollutants. That is why our work was aimed on synthesis and characterization of composite materials based on titanium dioxide and doped with sulfur and carbon with enhanced photocatalytic activity under UV and visible irradiation.

The powders were obtained using titanium(IV) ethylate, thiourea and carbon. Investigation of the obtained powders by means of energy-dispersive spectroscopy based on energy-dispersive technique proves that these materials include the elements Ti, O, C and S, uniformly distributed in the materials, no unexpected elements being detected. X-ray analysis revealed the phase of anatase in all the composites. It was established that composites consist of crystallites with sizes that vary from 10 to 20 nm. This is supported by studies using TEM.

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 with H1 or H2 types of hysteresis loop depending on the method of sample preparation. Predominance of pores up to 10 nm is characteristic of pure TiO_2, for composite samples C/TiO_2 this value is 5–35 nm, whereas for S/C/TiO_2 samples are up to 6 nm. S/C/TiO_2 samples demonstrate specific surface increase and average radius of pores decrease as compared to pure titanium dioxide and modified carbon.

Absorption spectra of nanocomposites showed a bathochromic shift as compared with the absorption band of pure TiO_2. The UV–Vis spectra reveal that the absorption edge from TiO_2 to S/C/TiO_2 is placed from 393 to 417 nm.

Nanocomposite samples S/C/TiO_2 showed higher photocatalytic activity in the destruction of safranine T under UV and visible irradiation compared to pure titanium dioxide. It may be connected with the participation of carbon and sulfur in the inhibition of electron–hole recombination, prolongation of charges lifetime, increasing of efficiency of interfacial charge separation.

Structure and thermodynamics of interactions in the nanocomposites based on PU/PHEMA matrix and nanofillers modified with aminoacids glycine and tryptophan

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The nanocomposites based on multicomponent polymer matrix consisting of polyurethane (PU), poly(2-hydroxyethyl methacrylate) (PHEMA), and nanofillers based on silica with mechanically activated surface and surface modified with aminoacids glycine and tryptophan are synthesized. The structure of the created nanocomposites and thermodynamic parameters of polymer matrix components interaction with nanofiller were studied.

The structure of the created nanocomposites was investigated by small-angle X-ray scattering and was shown that modification of densil surface by aminoacid glycine leads to an increase of average size of the particles and to the formation of a rough surface of filler. Introduction of modified nanofiller into polymer matrix influenced the structure of the matrix: there is a complete disappearance of the structural features of semi-IPN in the nanocomposites. With the introduction of the modified nanofiller into polymer matrix the mass-fractal of spatial distribution of the particles is preserved. However, the surface roughness of the particles increases because of the surface layer at the interface with the filler is formed, consisting of fragments of the polymer matrix.

The thermodynamic parameters of interaction between polymer matrix and nanofillers during process of formation of the nanocomposites were investigated. The free energy of interaction of densyl modified by aminoacid glycine or tryptophan, with polymer matrix, which is the semi-IPN with 17% PHEMA, is negative for all studied concentrations of nanofillers. With increasing the PHEMA content in polymer matrix from 17 to 37%, the value of the free energy of interaction between polymers and fillers became positive. This is the result of competition between two processes: the formation of dense surface layers on the surface of the filler, and the formation of interfacial layers with excess free volume in the polymer matrix which is semi-IPN with 37% of PHEMA.

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The study of artificial bionanocomposite protective layer for hatching eggs

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One of the important problem of modern poultry industrial is to effective prevent the deterioration of the quality of hatching eggs due to their secondary contamination by pathogenic organisms (viruses, bacteria, fungi) with the subsequent mass epidemic diseases of the number of birds [1].

The aim of our research was to improve industrial hatching technology by pre hatching treatment of hatching eggs with the «artificial cuticle» technology [2]. Technology is based on the formation on the surface of the hatching egg protective artificial film (cuticle) in accordance with the biomimetic principle [3]. The composition of the film includes chitosan as a matrix substance, titanium oxide (TiO_2), iron oxide (Fe_2O_3), zinc oxide (ZnO), silica (SiO_2) in the form of ultradispersed or nanoparticles, iron and copper sulfates, *etc*. Particularly successful application was the use of ZnO nanoparticles to impart antimicrobial properties and UV protection of surfaces of organic and inorganic substances. ZnO is also environmentally friendly and non-toxic substance which is also inherent photocatalytic activity. It is particularly important for the initiation photocatalytic processes of hydrogen peroxide (H_2O_2) formation. H_2O_2 can be used subsequently for aggressive destroying organic contaminants and disinfection of pathogens on the egg shell.

Proved that the use of the «artificial cuticle» technology for the protection of chickens hatching eggs enhances index of eggs hatchability on 4.0-18.1% with simultaneous decrease in the number of pathogenic organisms on the surface of eggs to 2.1- 4.7% of the initial number of bacterial colonies, and significantly enhances the quality parameters of chickens. The thermal characteristics of the protective layers of the native egg shell biomineral layers and artificial cuticles by means temperature-programmed desorption mass spectrometry technique (TPD-MS) has been studied.

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“Green” synthesis of CdS quantum dots by biological matrices

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Binary chalcogenides belonging to the groups II–VI semiconductors have attracted considerable attention due to their unique properties related to the size quantization effects. The preparation of CdS quantum dots (QDs) has been carried out using various methods: microwave heating, ultrasonic irradiation. However chemical methods are complicated, outdated, have low productivity and produce toxic wastes raising environmental safety. An alternative approach suggests the use of the biological systems for synthesis of QDs in order to produce nanoparticles at ambient temperature generating poisonous by-products. The purpose of our study was to develop green, fast and easy reproducible approaches for biological synthesis of CdS nanoparticles by bacteria, fungi and plant matrices, and characterize their structural, morphological and optical features. We have developed new reproducible methods of extracellular synthesis of stable CdS quantum dots using bacteria - *Escherichia coli*, the fungus - *Pleurotus ostreatus*, and plant - *Linaria maroccana* and *Nicotiana tabacum* [1-4].

Obtained CdS semiconductor QDs were determined by means of an UV-visible spectrophotometer, photoluminescence, TEM and electron diffraction analysis. Synthesized stable luminescent CdS nanocrystals possess absorption peaks at 362-464 nm, and luminescent peaks at 425- 500 nm. TEM of produced QDs revealed their size predominantly from 5 to 7 nm. Electron diffraction pattern confirmed the wurtzite crystalline structure of CdS QDs. Unique luminescent properties of studied CdS nanoparticles might promise their effective application for cell biology and biomedical research.

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Catalase mimetic activity of graphite decorated with nanoceria

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CeO_2 nanoparticles (nanoceria) has been reported to exhibit multiple enzyme mimetic activity (superoxide dismutase-, oxidase– and catalase–like). Its high catalytic activity is caused by the presence of surface defects and the ability of cerium to exist in two oxidation states Ce^{3+} and Ce^{4+}. The aim of this work is to study catalase mimetic properties of graphite decorated with nanoceria. Graphite – nanoceria composites were produced by the reaction of cerium nitrate deposition in the presence of graphite:

$4Ce(NO_3)_3 + 12NaOH + O_2 = 4CeO_2 + 12NaNO_3 + 6H_2O$.

The morphology of the nanomaterials was studied by scanning electron microscopy (SEM, MIRA3 LMU, TESCAN instrument with a resolution of 1 nm, Fig.).

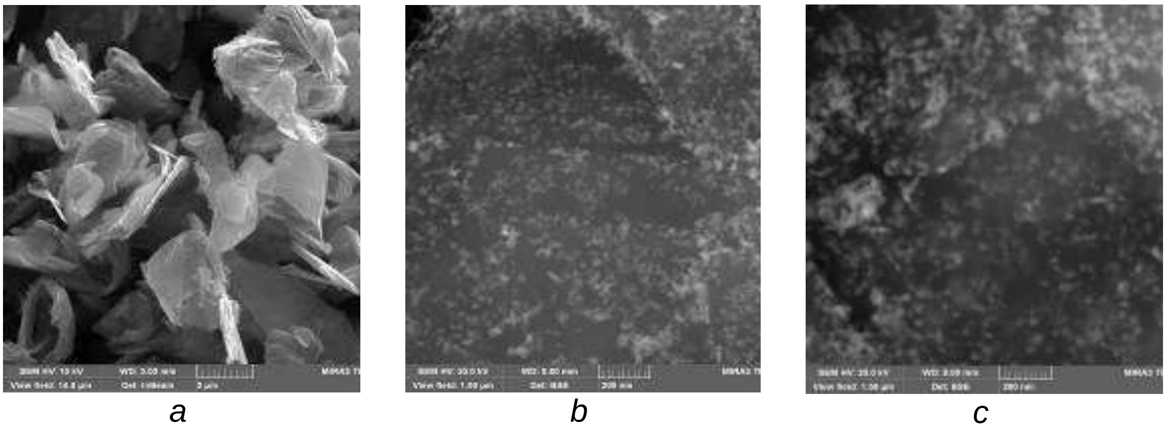

Fig. SEM images of materials: pristine graphite (*a*), modified graphite with 12 % (*b*) and 20 % (*c*) of nanoceria

Catalase mimetic activity of nanocomposites, pristine graphite and nanoceria was studied in the reaction of H_2O_2 (~1 – 10 %) decomposition at room temperature and pH from 8 to 11. To obtain the kinetics data, the volume of released oxygen was measured. Enzyme mimetic activity of the materials was evaluated using the Michaelis constant (K_M) that was calculated from Lineweaver – Burke plot.

The results showed an extremal correlation between enzyme mimetic activity and pH–value for nanoceria and nanoceria-containing nanocomposites.

Quarts glass with mono and double doped Cu and Cu-Eu nanospecies as advanced optical materials

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Transition ions proved to be very promising dopants for elaboration of multifunctional materials – effective photo-, X-ray- and thermoluminophors, scintillators, *etc*. [1, 2]. Quite recently we reported on cerium and europium nanospecies in quarts glass [3]. Here we present spectral study on copper and copper-europium nanospecies in quarts glass.

The set of samples with different content of Cu-, Eu- in quartz glass: *1* - Cu(0.05 %)/SiO_2, *2* - Eu(0.05 %)/SiO_2, *3* – Cu(0.025 %),Eu(0.05 %)/SiO_2, *4* – Cu(0.05 %),Eu(0.05 %)/SiO_2, *5* – Cu(0.05 %),Eu(0.025 %)/SiO_2 were prepared using modified sol-gel method [3]. The main results are as follows:

1) UV-Vis absorption spectra of Cu/SiO_2 and Cu,Eu/SiO_2 consist of two kinds of bands – very intensive and broad bands in the range of 220-250 nm and the next ones 290-300 nm. The first kind of bands was attributed to CT transition $O^{2-}\rightarrow Cu^{2+}$ ions while the next ones we assigned as transition $3d^9 4s \rightarrow 3d^{10}$ of Cu^{1+} ions. The presence of Cu^{2+} species in the samples is evident also from the spectra in the range of 600-900 nm. In this range are observed very weak bands – typical for forbidden crystal-field *d-d* transition of Cu^{2+} species

2) Photoluminescence (excitation-emission) spectra of Cu/SiO_2 and Cu,Eu/SiO_2 display bands in the range of 250-350 nm and 500-560 nm, respectively, which are caused by $3d^9 4s \leftarrow 3d^{10}$ of site-dependent Cu^{1+} ions.

3) Photoluminescence spectra of Eu/SiO_2 and Cu,Eu/SiO_2 exhibited fine line structure arising from $^5D_0\rightarrow{}^7F_n$ manifolds (570–750 nm) of Eu^{3+} ions. Domination of the $^5D_0\rightarrow{}^7F_2$ transition in the spectra clearly points on low site symmetry of Eu^{3+} ions.

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Sorption performance of ethylene glycol dimethacrylate and methacrylic acid copolymers with different cross-link ratios towards rare earth elements

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Due to their unique properties, rare earth elements (REEs) have found widespread application in the different fields of material science such as magnets, alloys, phosphors, catalysts, *etc*. [1]. Therefore determination of REE content in different materials is the challenging issue. The main difficulty is complex matrices or high concentrations of concomitant REEs.

To solve these problems, separation of REEs from the matrix and their preconcentration are needed in most cases. Adsorption allows to facilitate these procedures due to its high efficiency, rapidity, simplicity, and low cost.

Among the diversity of sorption materials, synthetic ion-imprinted polymers should be emphasized. They are synthesized by copolymerization of functional and cross-linking monomers in the presence of the target ion. It causes the selective recognition cavity formation in the polymer network [2].

Synthesis of blank polymers is an integral part of any experiment in imprinting. Such polymers are obtained under the same conditions but with no addition of the target ion. They are always considered only as control materials. Nevertheless, their rigid porous structure offers great opportunities to investigate them as independent efficient sorption materials.

In the present work, ion-imprinted and non-imprinted copolymers of ethylene glycol dimethacrylate and methacrylic acid with different cross-link ratios were synthesized via free-radical bulk polymerization. Gadolinium has been chosen as the imprinted ion, Alizarin red S – as the complexing agent. It was shown that obtained materials have the potential to be applied in selective extraction of rare earth ions from aqueous solutions. The sorption properties of these materials under different experimental conditions were investigated. pH value of 6 was found to be the optimal acidity for REEs recovery. Adsorption isotherms were recorded for all materials under study. The maximum sorption capacity was calculated to be about 40 mg/g.

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Comparison of drugs efficacy on the basis of silica nanoparticle in the treatment of maxillofacial region inflammatory diseases

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The problem of treatment of maxillofacial region inflammatory diseases remains one of the most actual problems of dentistry. We have developed a new method for the treatment of inflammatory diseases based on the use of nanodispersed silica drugs with cationic surface active antiseptics, directional antimicrobial drugs transport in area of inflammation and immunomodulatory therapy.

The aim of the study was to substantiate the efficiency of the developed method for management of pyo - inflammatory diseases.

Developed method for the treatment of inflammatory diseases was assessed through the results of treatment 67 patients with phlegmon of maxillofacial region, which were divided in two groups of patients representative by pathology, age, sex, and concomitant diseases. After operation both groups get treatmen, but in the study group (32 patients) it was held according to developed methodology and in the comparison group (35 patients) – by traditional method. Evaluation of treatment efficacy was performed according to clinical, laboratory, microbiology, cytology and statistical methods.

The indicators which were estimated showed that in the study group their normalization were more quickly than in the comparison group. Inflammation almost completely disappeared on 5th day of observation, refined wounds of necrotic tissue appeared bright red granulation, bacterial contamination of wounds was below a critical level, allowing to impose secondary seams. While in the comparison group even on 6th day of observation was pale granulation tissue and wound partially filled in tsytohramah determined degenerative modified leukocytes and neutrophils with incomplete phagocytosis. Microbial contamination of wounds was significantly higher than in patients of study group. In this group of patients only on 7-8th day was completing first phase of wound healing, and it led to longer patients hospitalisation.

Treatment of purulent - inflammatory maxillofacial areas diseases by the developed method ensures uncomplicated postoperative period and allows to reduce duration of patients hospitalisation.

Structural and surface properties of biocomposite protein/mesoporous silica

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Protein–surface interactions are intensively investigated with regard to wide applications of biocomposite materials as well as in the field of nano-biotechnology and materials science (biomedical implants, biosensors, biochips, therapeutic nano-devices, drug delivery systems) [1,2]. The physicochemical, structural and morphological properties of material are important in adsorption process (speed, efficiency and selectivity of adsorption) of biomolecules on its surface as well as protein-surface interactions (adhesion, stable interaction of adsorbent/adsorbate) [3]. Mesoporous silica materials due to their desirable and unique properties as well as possibility of functionalization and changing the surface morphology (texture, roughness, porosity, geometry) during their synthesis are very attractive group of adsorbents which can be useful as carriers of compounds showing biological activity.

The paper presents the results of the Lysozyme (LYS) adsorption on the series of mesoporous silica materials with various porosity and pore sizes. The physicochemical and structural properties of the protein/silica support were determined by the nitrogen adsorption/desorption isotherms and the X-ray diffraction scattering patterns (SAXS). The micro- nanostructure and morphology (texture, micro- nanoroughness, homogeneity) of the MCF surface with adsorbed protein layers was carried out using the atomic force microscopy (AFM) and the optical profilometer (OP). Moreover, the topography (structure imaging), composition and distribution of elements (chemical maps) on the composite surface of lysozyme/silica system were studied by using the scanning and transmission electron microscopy with X-ray microanalysis (SEM/EDS, TEM/EDX).

Acknowledgements
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UV-Vis DRS and ATR-FTIR spectroscopic studies of porous MCF silica surface with adsorbed lysozyme

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With increasing use of biomolecules, especially proteins, in many different applications, ranging from pharmaceuticals to biomaterials and biosensors, there has appeared a need for detailed analysis of protein adsorption at a solid interfaces and its behavior and interaction with sorbents surfaces [1].

In this work, the interactions between protein (LYS) and the porous MCF silica surfaces (mesocellular foam) have been investigated. The MCF silica materials were prepared by using the non-ionic triblock Pluronic copolymers as a template, according to a modified procedure described in the paper [2].

The UV-Visible diffuse reflectance spectroscopy (UV-Vis DRS) was applied to study the structures of prepared protein/silica supports. The analysis with DRS UV-Vis spectroscopy showed existence of protein molecules on the MCF surface (well known absorbance maxima for LYS at near wavelengths ~280 and ~220 nm, respectively). The spectrum maximum of LYS situated at ~281 nm is due to the $\pi \rightarrow \pi^*$ transition of the aromatic amino acids tryptophan (Trp) and tyrosine (Tyr) and to a small extent, to the absorbance of cystine (i.e. disulfide bonds). On the other hand, the maximum of spectrum at ~230 nm is attributed to the $n \rightarrow \pi^*$ transition of the carboxylic group in peptide bond [3]. Additionally, the changes in bonding properties introduced by adsorption of protein molecules on the mesoporous silica support, and physical interactions between the protein molecules and silica surface were monitored by using ATR-FTIR infrared spectroscopy. ATR-FTIR data before and after the LYS adsorption confirmed the presence of the adsorbed protein on the surface of porous material. It was observed that protein/silica composite on the ATR-FTIR spectrum exhibits the peak-I located at 1654 cm^{-1} for the amide-I band and the peak-II located at 1532 cm^{-1} for the amide-II band [4].

Acknowledgements
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Thermochemical synthesis of luminescent materials in the Y_2O_3–ZnO system doped with Eu^{3+} ions

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Nanostructured powders of yttrium-zinc oxide doped with europium ion, Y_2O_3–ZnO:Eu^{3+}, were synthesized on the basis of zinc-modified Y_2O_3 matrix (red phosphors) by the method of thermochemical reactions (combustion) using nitrate salts of yttrium, zinc, and europium in the presence of saccharose as a fuel. Y_2O_3–ZnO:Eu powders were thermally treated at 700–1100°C in an oxidizing medium (air). An analysis of the luminescence spectra of the Y_2O_3–ZnO:Eu system led to a conclusion that the emission intensity of the samples under excitation at 467.7 nm largely depends on the treatment temperature of the precursor. The main peak observed under excitation of the phosphor is the luminescence at 611 nm, associated with the supersensitive electric-dipole transition $^5D_0 \rightarrow {}^7F_2$, and the luminescence intensity of the main peak becomes five times higher upon treatment in the range from 700 to 1100°C (Fig.).

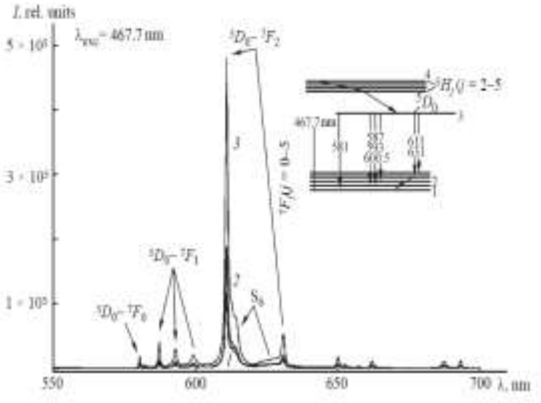

Fig. Luminescent spectra Y_2O_3–ZnO:Eu^{3+}:
1 – 700, *2* – 900, *3* – 1100 °C

An yttrium-zinc oxide ceramic was formed from powders calcined at temperatures of 700, 900, and 1100°C. With Y_2O_3–ZnO:Eu^{3+} powders calcined at 700°C used for compaction of a ceramic, a semitransparent light yellow ceramic is formed with grain size of 2–3 μm, whereas the ceramic obtained by treatment of the precursor powders at temperatures of 900 and 1100°C is less dense and nontransparent and has a grain size of 5–10 μm. The semitransparent ceramic exhibits a photoluminescence emission in the red spectral range at 610 nm under excitation at a wavelength of 468 nm. This composite ceramic may be promising as a material for solid-state photoluminescence converters of the emission from a blue light-emitting diode to the red spectral range and can serve as a basis for red lighting devices (lighting and alarm systems).

Simulation of adsorption complexes of 2-hydroxyethyl methacrylate on silica surface

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Poly(2-hydroxyethyl methacrylate) (PHEMA) is considered as a promising material for application in medicine. One approach to creating new materials based on PHEMA can be the filling with nanosilica covered by biologically active substances. In this aspect, it is necessary to study the interaction of this polymer with silica surface. An effective tool for this purpose realized in the presented work is the computer simulation.

It is known that the adjacent side atomic groups of monomer unit (Fig., *a*) of PHEMA are capable to form hydrogen bonds with each other, so for simulation of adsorption complexes the dimeric unit $(HEMA)_2$ is used. As a model of silica surface, the cubic cluster of the gross formula $Si_8O_{16}H_8$ was elected. This structure is similar in size to $(HEMA)_2$ and does not require introducting pseudoatoms into the periphery of the cluster to compensate for boundary effects.

All the calculations have been carried out by means of the GAMESS US program by density functional theory (DFT) method with functionals B3LYP and basis set 6-31G(d, p).

According to the results of calculations, in the adsorption complex the carbonyl groups (C=O) of $(HEMA)_2$ associated by hydrogen bonds with silanol groups of silica surface (Fig., *b*). Hydrogen atoms of silanol groups retard a part of the electron density from the oxygen atoms of carbonyl groups and weaken the covalent bonds C=O. The calculations are in a good accordance with the results of an IR spectroscopy examination.

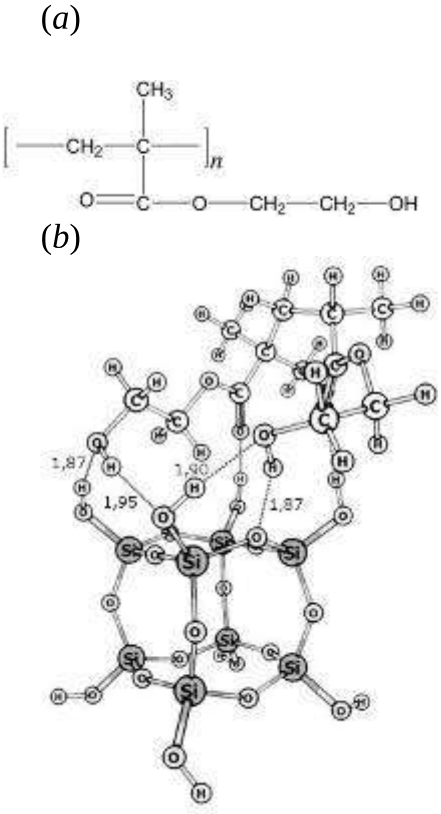

Fig. Monomer unit of poly-HEMA (*a*) and the possible structure of adsorption complex of $(HEMA)_2$ on the silica surface (*b*). The bond lengths are indicated in Å

Sol-gel synthesis and characterization of hybrid organic-inorganic membranes

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Hybrid organic-inorganic materials find increasingly wider application. The composition of such material determines the membrane properties and ultimately its practical application. Hybrid membranes with varied composition of polymeric matrix and constant content of inorganic counterpart (20 wt. % of sol-gel system) were synthesized via photo-initiated polymerization and *in situ* sol-gel process. To create polymeric matrix mixture of monomers: acrylonitrile (AN)-acrylamide (AAm)-3-sulfopropylacrylate potassium salt (SPAK) was chosen. The composition and chemical structure of synthesized films were investigated by ATR-FTIR spectroscopy.

Table. Composition of hybrid organic-inorganic membranes

Sample	PS1	PS2	PS3	PS4	PS5	PS6	PS7
AN, wt.%	8.5	17.0	25.7	34.2	42.6	51.1	59.5
AAm, wt.%	65.2	56.7	48.0	39.5	31.1	22.6	14.2
SPAK,wt.%	26.3	26.3	26.3	26.3	26.3	26.3	26.3

The spectra shown in Fig. 1 are typical for major component AAm. The bands at 3410 cm^{-1} $\nu_{as}(NH_2)$, 3190 cm^{-1} $\nu_s(NH_2)$, 1655 and 1612 cm^{-1} are characteristics of AAm unit. The presence of a band at 2243 cm^{-1} in spectra indicates a fraction of CN group from AN. It can be noticed a good correlation between theoretically expected and experimentally observed absorption of AN and AAm characteristic bands (Fig. 2). The bands at 1655 and 1612 cm^{-1} are decreasing with the reduction of AAm content, whereas the band at 2243 cm^{-1} rises with increasing of AN content. Furthermore, the spectra shown reveal absorption band at 982 cm^{-1} ν(Si-O) which proves the presence of inorganic component in all samples.

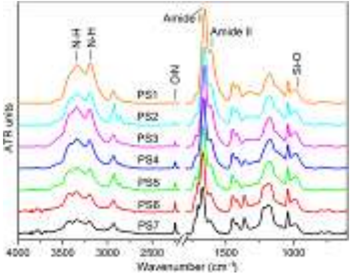

Fig. 1. FTIR spectra of hybrid organic-inorganic membranes with varied monomer ratios

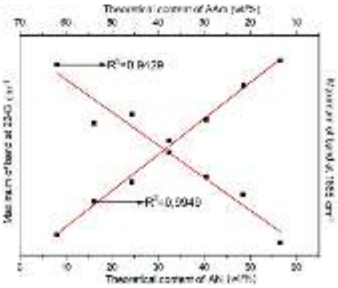

Fig. 2. Correlation between C≡N band and Amide I band *vs* monomer feed content

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Adsorption properties of chitosan-silica composites towards selected dyes

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Hybrid inorganic-organic materials based on natural polymers are very promising adsorbents regarding their high sorption affinity towards various substances and low costs [1,2]. These composites show high selectivity and capacity, and fast kinetics which may be a crucial factor in technological applications. Among these materials the chitin and chitosan hybrid mesoporous composites are very promising for dyes removal from waters and wastewaters.

The chitosan-silica composites were synthesized by impregnation and sol-gel methods. The surface and structure properties were investigated by SEM/EDX, FTIR, adsorption/desorption of nitrogen, and potentiometric titration. The composites are differentiated with regard to grain size, chemical composition, specific surface area, pore size and volume, surface morphology, and acid/base properties. Due to polycationic structure of chitosan the obtained composites reveal high adsorption affinity towards dyes, and their sorption effectiveness depend on physicochemical, surface and structure properties.

The measurements of adsorption isotherms and concentration profiles were carried out for selected anionic azo dyes in aqueous solutions. The experimental equilibrium and kinetic data were analyzed by using various equations and models. The influence of surface and structure characteristics of the composites and adsorbate properties on adsorption capacity and rate was investigated. In the case of microporous composite partial inaccessibility of its internal structure for dye molecules was found, moreover, in this case the adsorption process was the slowest and controlled by a diffusion rate into pore space. Strong relations were found between adsorbent surface charge, content of chitosan, pore size, hydrophobicity/hydrophilicity, adsorbate molecular size and functional groups, presence of impurities and adsorption.

Acknowledgements

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Hybrid composites and their application for removal of sulfonated azo dyes from aqueous solutions

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Physical, chemical and biological techniques have been proposed for removing dyes from wastewaters including chemical oxidation, membrane separation, coagulation, photocatalytic degradation, electrochemical, adsorption, and microbial degradation. Among these techniques adsorption shows the best results as it can be used to remove different types of coloring substances. Many commercial systems use activated carbon because of its excellent adsorption ability, however, it is relatively expensive. In order to decrease the cost of adsorption treatment, attempts have been made to find inexpensive alternative adsorbents like chitin or its derivative, chitosan. These biopolymers have particular structure, physicochemical characteristics, chemical stability, high reactivity and excellent selectivity towards aromatic compounds, due to presence of chemical reactive groups in polymer chains which can interact by physical and chemical forces [1,2].

The aim of the present work is comparison of the physicochemical and adsorption properties of three types of chitosan-silica composites: materials obtained by impregnation of silica gel and fumed silica with chitosan, and material synthesized by sol-gel method. Various techniques were used for their physicochemical characterization: FTIR, SEM/EDX, thermal analysis, elemental analysis, nitrogen adsorption/desorption, potentiometric titration. In order to verify their adsorption properties towards selected anionic azo dyes the equilibrium and kinetic experiments were carried out for aqueous solutions. The adsorption isotherms were analyzed by using the theory of adsorption on energetically heterogeneous solids. The kinetic data were analyzed by using simple equations like pseudo first- and pseudo second-order, and multi-exponential as well as diffusion models. The correlations between adsorption capacity and adsorption rate, composite and dye properties were found.

Acknowledgements

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Preparation of fine dispersed sodalite by hydrothermal modification of natural clinoptilolite

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Formation of new mineral phases by hydrothermal crystallization of natural aluminosilicates is actual, first for determination of zeolite-forming regularities going on in alkali-aluminosilicate systems of zeolite-forming, and second, for creation of analogues of zeolite minerals rare in the nature.

The research aimed to create fine-dispersed, characterized by high purity and corresponding chemical composition reference sodalite on the basis of natural material, clinoptilolite-containing rock, in a low temperature crystallization regime.

Our experiment was based on the method recently developed for zeolite synthesis from alkali aluminosilica gels. The object of the study was clinoptilolite-containing rock from Georgia-CtR. For decationizing and elevation of SiO_2 reaction ability it was treated in 1 N HCl solution. CtR crushed to powder was placed in Teflon flasks and treated in water bath at periodical shaking terms. Mineralizing agent was used in various concentrations, up to 10–30% NaOH-solution. Direction of clinoptilolite-containing rock crystallization in a wide time interval (from 20 to 100 h) and the phase purity of the obtained samples were checked by XRD powder patterns. By the same method we determined that in 20 % NaOH-solution sodalite crystals are formed, which preserve structure for 70 h. Ready product was washed by distilled water till constant pH (8÷9) value and then dried at 105–110°C in a thermostat. We determined composition of the obtained fine-dispersion sodalite on the base of the data and it conforms to the chemical composition of the main sodalite, that is, hydrosodalite:

$$Na_{6.35}[Si_{7.01}Al_{5.85}O_{24}].5.92H_20$$

Adsorption capacity to water vapor p/p_s=0.40 was determined and at 18°C terms 4.2 mmol/g. Thus, on the basis of the studies carried our, it can be stated that the product with sodalite structure can be obtained by crystallization of natural mineral. Sodalite formation is realized by a simple method, from the cheap, easily accessible natural raw material.

Enzyme mimetic activity of nanosized cerium dioxide following different surface modification

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During last decade, cerium dioxide nanoparticles attracted significant attention of researchers because of their unique regenerative redox properties, which are attributed to Ce^{3+} / Ce^{4+} surface ratio [1]. Potential biomedical application of cerium oxide-based nanostructures is of particular interest due to their catalytic activity resembling those of major antioxidant enzymes that control free radical metabolism in living systems [2]. Thereat superoxide mimetic activity is attributed to high Ce^{3+} content and catalase mimetic-one – to prevalence of Ce^{4+} at the nanocrystallite surface [3].

The objective of our work was to assess enzyme mimetic activity of wet chemistry – obtained cerium oxide nanoparticles after surface modification by alkaline or peroxide treatment.

Cerium dioxide nanoparticles were formed during cerium oxide dissolving in nitric acid with consequent sedimentation by alkaline solution. The resulting suspension was heated and centrifuged. Then dehydrated nanoparticles were treated by ammonium hydroxide or hydrogen peroxide to modify the ratio between surface cations of tri- and tetravalent cerium.

To assess the enzyme mimetic activity we exploited inhibition of luminol-enhanced chemiluminescence under the influence of the two nanosized cerium dioxide modifications using superoxide dismutase and catalase solutions as a reference.

Both modifications of cerium dioxide nanoparticles have demonstrated ability to decrease the intensity of luminol-derived chemiluminescense similar to those of superoxide dismutase, though less powerful. The effect was higher in the case of the hydrogen peroxide-treated nanoparticles and became somewhat weaker after the adding of catalase. Although lower expressed, inhibition of the chemiluminescense by cerium dioxide nanoparticles treated with ammonium hydroxide was not affected after the catalase adding.

Conclusion: different modification of cerium dioxide nanoparticles aimed to vary Ce^{3+} / Ce^{4+} surface ratio results in altered enzyme mimetic activity with prevalence of either superoxide dismutase- or catalase-like catalytic activity.

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Interaction of magnetite nanoparticles with negatively charged dyes

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Magnetite (iron oxide) nanoparticles are widely used as controlled carriers for drug transportation. To ensure the targeted delivery of drugs, their complexes with nanoparticles must be stable. Until present time, studies of nanoparticle-drug complex stability have mainly had a qualitative character. Therefore we propose a method of quantitative estimation of the complex stability by analyzing the thermodynamic binding parameters, in particular, the drug-nanoparticle binding constant value.

In this work we present the binding constants of food dyes (eosin, tartrazine and fast green) with magnetite nanoparticles. Since these dyes are negatively charged and, thus, are able to electrostatically interact with the positively charged surface of magnetic nanoparticles, they were used as model objects for approbation of the proposed approach for assessing the complex stability.

The calculation of binding constants was carried out using spectrophotometric titration data. The nanoparticle suspension was added to aqueous solutions of dyes to get different magnetite/dye concentration ratios and then dispersed using ultrasonic disperser UZDN-2T. The obtained colloid solutions were placed on the samarium-cobalt magnet in order for nanoparticles with bound dye to precipitate. Absorption spectra of the supernatant were registered by spectrophotometer Specord M40 (Germany). The absence of magnetite in the supernatant was controlled by the absence of their absorption band at 340 nm. Thus, spectra of only free dyes were recorded. The decrease in the intensity of absorption spectra with the increasing relative concentration of nanoparticles was observed in all systems. It indicates a decrease of the free dye concentration due to the formation of dye-nanoparticle complexes. The Langmuir model of equilibrium binding was applied to obtain dye-magnetite binding constant from experimental data. It was assumed that statistical distribution of the ligand molecules upon binding to the nanoparticle surface can be neglected. The calculation was performed with and without cooperativity factor. The calculated binding constants indicate that interactions of nanoparticles with the investigated dyes have both electrostatic and hydrophobic nature.

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Soil recultivation by natural nanoporous materials

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The world practice for recultivation work possesses the various methods of restoration of soil and water ecosystems. Pollution by oil and oil products leads to the significant changes in the physico-chemical properties of soil and destroys the water-air mode. More and more farmers are turning to the use of non-traditional mineral-raw material resources as fertilizer, including such nanoporous materials as natural zeolites, deposits which are found in Georgia.

The impact of nanoporous zeolite containing tuffs (clinoptilolite) introduced into the oil polluted soil has been studied in the work of the biometric indicators of winter wheat.

Table. Energy of germination and seed emergence of wheat on the options of the experiment

Biometric indicators	Crops	Options for the experiment					
		The soil (control)	Soil + Zeolite (substratum)	The degree of soil contamination from mass of the soil			
				Soil + 5% of oil	Soil + 10% of oil	Soil + zeolite + 5% of oil	Soil + zeolite + 10% of oil
		I	II	III	I V	V	VI
Energy germination	1 plant	70	81	-	-	10	-
	2 plant	80	90	30	5	60	40
Germination	1 plant	85	90	-	-	55	30
	2 plant	90	96	50	35	75	55

Analysis of the tabular data of the first and second crops shows that the introduction of the zeolite in the soil has a positive impact on the energy germination and the germination of plants.

It has been shown that the natural zeolites by their specific properties can be considered as a promising adsorptive material preventing migration of polluting hydrocarbons in the layers of soil and contributing to the increase in the biodegradation of the pollutant in the processes of treatment and restoration of the soil.

Immobilization of luminescent Eu(III) *β*-diketonato-1,10-phenanthroline complexes on aerosils

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Covalent and non-covalent immobilization (sorption) of adducts of Eu(III) *tris*-*β*-diketonates and 1,10-phenantroline on A300 and A380 aerosils was carried out. Three different types of sorption isotherms according to Giles classification were obtained: Henry isotherms (C-type) for ligands containing alkyl substituents; S-type isotherms in the case of aromatic *β*-diketones and L-type – for molecules with trifluoromethyl groups. The highest values of sorption were observed for complexes with acetylacetonate and dipivaloylmethane, intermediate values – for benzoylacetonate and the smallest – for the complexes with aromatic and fluor-containing ligands. It was shown that the growth of electron-accepting ability of *β*-diketones leads to a decrease of sorption. Covalent immobilization of Eu(III) complexes was carried out through modification of their molecules with anchorage of triethoxysilyl groups.

In previous reports we studied luminescent complexes of Eu(III) in the hybrid materials and proposed spectral criteria for evaluation of the uniformity of molecules distribution in matrix and the degree of their association [1]. The proposed criteria were used to analyze the environment of complexes on aerosil surface. Thus, the widened emission spectra, concentration quenching upon the growth of sorption and low values of the «red-orange» ration (ratio of the intensity of Eu(III) electric and magnetic dipole transitions) for covalently anchored complexes indicated that their molecules are uniformly distributed on the surface of aerosils and do not form associates. So, they form a uniform monolayer. In non-covalent attached (adsorbed) complexes the opposite behavior was discovered: the narrow-line emission spectra were close to those of crystalline complexes, the linear form of the dependence of the intensity *vs*. sorption and the high values of the «red-orange» ration indicated a significant association of their molecules on the surface of aerosils. This phenomenon can be considered as polymolecular sorption.

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Surface composition effect of Ni-Fe catalysts in the reaction of CO_2 methanation

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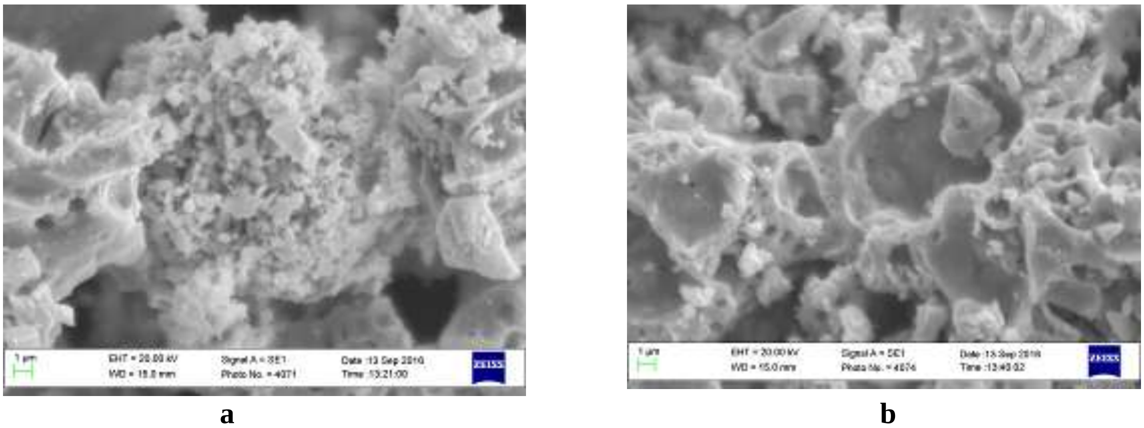
The series of the Ni-Fe catalytic system with different metal ratio (Ni:Fe 100:0 to 65:35) were prepared by coprecipitation method with NH_3 as a precipitation agent. All samples were reduced by He+H_2 mixture from oxide form to the metal state and then they were used in methane production from CO_2 and H_2.

Investigation of catalytic activity of Ni-Fe systems in the reaction of CO_2 methanation was performed. It was found that $Ni_{80}Fe_{20}$ catalyst with the highest specific surface (16 m^2/g) showed the best performance at 300–500°C with 62 % of CH_4 yield. $Ni_{75}Fe_{25}$ sample with lowest specific surface (2 m^2/g) showed the worst catalytic performance in terms of CO_2 conversion and CH_4 yield (14 %).

TPD MS analysis of active and non-active samples' surface showed that methanation process onto Ni–Fe catalysts has the mechanism that doesn't involve oxygen-containing intermediates.

The surface of active ($Ni_{80}Fe_{20}$) and non-active ($Ni_{75}Fe_{25}$) catalysts was investigated with SEM (Fig.). SEM-EDX analysis showed that the elementary composition of the $Ni_{80}Fe_{20}$ is close to the calculated one. For the $Ni_{75}Fe_{25}$ elementary composition is uneven, in the range of: Ni 30-86 at. %, Fe 22-61 at. % and O 1-11 at. %.



a b

Fig. Scanning electron micrograph of the samples: (*a*) - active $Ni_{80}Fe_{20}$, (*b*) non-active $Ni_{75}Fe_{25}$

It could be concluded that the chemical composition of the Ni-Fe catalysts' surface layer has a high influence for their catalytic activity in the reaction of CO_2 methanation.

Localization of the standard Reichardt's indicator in micelles of ionic surfactants from MD simulations

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Molecular dynamics simulation method was applied for the direct investigation of localization and orientation of the standard Reichardt's solvatochromic indicator in micelles of sodium dodecyl sulfate (SDS) and cetyltrimethylammonium bromide (CTAB). Simulation results proved the localization of the indicator on surface of these micelles (i.e. in the Stern layer).

The average angle 'micelle center of mass — N atom — O atom' equals 114° on SDS micelles and 104° on CTAB micelles, which means that in the first case the oxygen atom is pushed towards water phase somewhat farther than in the second case. For detailed characterization of the location of the indicator the average number of surfactant C and H atoms, located in vicinities of different parts of the molecule, N_{CH}, was calculated. For a given atom this quantity is determined by depth of immersion in the micelle hydrocarbon core, therefore a set of N_{CH} values describes the orientation of the whole molecule. Calculations were performed for O and N atoms and for each phenyl substitute. The N_{CH} values for symmetric substitutes were averaged.

It was found that, for all groups except *ortho*-substitutes at the pyridine ring, N_{CH} differs significantly on SDS and CTAB micelles. This allows one to conclude that the difference in experimentally measured polarity parameters $E_{\mathrm{T}}(30)$ of these micelles to the considerable extent is caused by different orientation of the indicator molecule. The time-averaged molecule orientation is depicted in Fig. Average rotation angle of the molecule plane around N–O axis is 35 and 38° in SDS and CTAB, respectively. These results agree with the fact that in SDS solution, the $E_{\mathrm{T}}(30)$ value is higher than in CTAB solution [1].

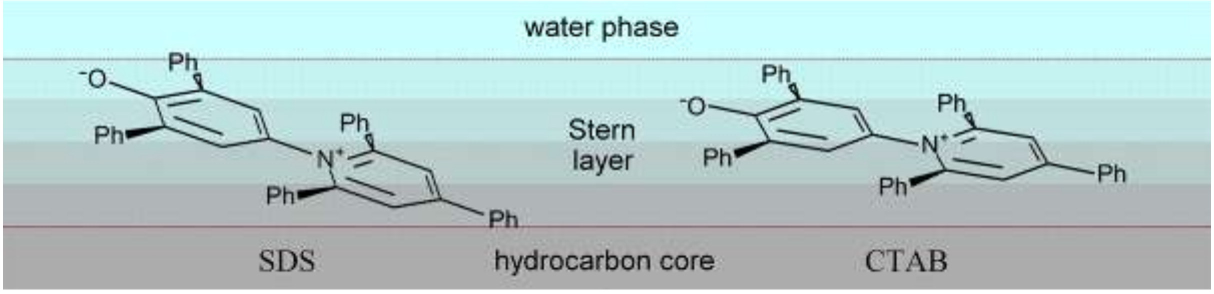

Fig. A schematic representation of the orientation of the indicator molecule on micelle surfaces

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Antibacterial and antiviral activity of nanostructured composites with silver nanoparticles

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Particular attention is paid to the creation of biologically active nanocomposites (NC), including silver nanoparticles (NPs). Such compounds can be promising for medicine. Of particular interest is the vapor deposition method, from the vapor phase (EB-PVD). This method allows one to control the rate of evaporation and the density of the vapor stream, as well as the amount of evaporated matter. This method eliminates the need to use stabilizers and reducing agents in the process of obtaining metal NPs and avoids the need for further purification of the particles. It is known that in most applications of NP, such as microelectronics, medicine, spectroscopy, even the smallest impurities are unacceptable. With the EB-PVD method, NC was obtained with NPs silver on the surface of granules of a medical substance - aminocaproic acid (ACC). The obtained nanostructured objects were studied using laser correlation spectroscopy, scanning electron microscopy and analyzed with the help of a complex of computer image processing software and statistical data "Image-Pro Plus version 6.0" and "Statgraphics". Data on the dimensions of NPs are in good agreement with the results, from the broadening of X-ray diffraction patterns and microphotographs. Nanocomposites contain particles in the range from 10 to 70 nm with a maximum of 20-28 nm, the particles have a predominantly spherical shape. Cytotoxic properties of ACC matrix and nanocomposites of ACC with nanosilver were determined of the culture infusoria *Colpoda steinii* and in the tissue culture of the chorion-allantoic membranes of 11-14 day-old chick embryos (CAO). All the drugs studied were non-toxic at a dose of 25 mg/ml. The anti-influenza activity of the drugs for human influenza viruses A/Hong Kong/1/68 (H3N2) and A/PR/8/34 (H1N1) *in vitro* was studied. The results indicate that the nanocomposite with the highest content of silver particles (0.084%) inhibited the reproduction of both influenza viruses in the culture of CAO by more than 2.0 lg TID50 compared to the ACC matrix. Studies of the antibacterial activity of nanocomposites have shown that they have antibacterial activity against strains of *Staphylococcus aureus* ATCC 25923 and *Staphylococcus aureus* 2781. Antibacterial activity nanocomposites of ACC with nanosilver are significantly higher than that of the ACC matrix.

Nanosized Pt/SnO_2 materials and perspectives of their use in adsorption semiconductor sensors

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Nanosize oxide semiconductor materials are widely used in adsorption semiconductor sensors as main components of gas sensitive layers. Devices based on such sensors have successful combination of high response, good dynamic properties, low power consumption, small size, low weight and can work in a wide range of environmental temperature. Among the gas sensitive materials the most popular is tin dioxide due to its low cost, sensitivity to the surface process in a temperature range 100-650 °C where the molecules adsorbed on the surface are engaged in chemical reactions and due to presence of free electrons in the semiconductor conduction band, oxygen vacancies and chemisorbed oxygen on the surface [1]. However, the responses of such sensors for some of the most common gases such as methane are negligible. This problem can be solved by using semiconductor particles with sizes less than 10 nm (due to size effect the response should increase [2]) and introduction of active catalytic additives. For methane oxidation reaction platinum is known to be one of the most active catalysts [3]. The aim of this work was to study nanosized Pt/SnO_2 nanomaterials as a base of the gas sensitive layers for the adsorption-semiconductor sensors to methane.

It has been shown that introduction of platinum to nanosized tin dioxide leads to significant increasing of the sensor response to 930 ppm CH_4 (7–8 times) compared to unmodified SnO_2 and lowering temperature of 10% methane conversion from 466 °C for SnO_2 to 373 – 418 °C for Pt/SnO_2 depending on Pt loading. This result is in agreement with a role of the catalytic oxidation of target gas by chemisorbed oxygen on the gas sensitive layer as one of the key stages in the formation of the sensor response [4]. It was found that the obtained Pt-containing sensors have also good dynamic properties: response time is equal to 7 s and relaxation time is equal to 16 s. The long-term stabilities of the sensors were investigated during 3 months and no significant changes in their properties were found. The created sensors are perspective to use them in devices for detecting methane leakages in e.g. households or coal mines.

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Ionization of flavonols in mass spectrometric experiment

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Flavonols are well-known compounds of plant origin with the antioxidant activity resulting from their ability to inhibit free radicals. To improve the efficiency of original flavonol, its derivatives with the electron-donating groups grafted to the side aromatic ring of the molecule were synthesized.

Laser desorption/ionization mass spectrometry (LDI MS) and quantum chemical methods were used to characterize flavonol (L1) and its derivatives (4'-(N,N-dimethylamino)flavonol, L2, and 4'-[N,N-di(2-hydroxyetylamino)]-flavonol, L3) molecules.

Proton/electron affinities, ionization energies, proton/electron detachment energies for initial flavonols molecules and for their ions resulting from proton/electron capture or loss were calculated. Mechanisms of flavonols ion formation were analyzed. The results obtained indicate the correlation between the LDI MS data and the parameters calculated. For example, the L2 molecule is characterized by the lowest energy of electron affinity and has the weaker $L2^{-}$ ions peak than $L1^{-}$ and $L3^{-}$ ones (Fig.). This indicates that L1 and L3 compounds will easier capture an electron from free radicals. The lowest value of the hydrogen detachment energy is observed for L2 molecule; this compound has a peak $[L2\text{-}H]^{+}$ in mass spectra while two others flavonols have not. The L2 compound is the most active in the reactions with radicals via hydrogen transfer.

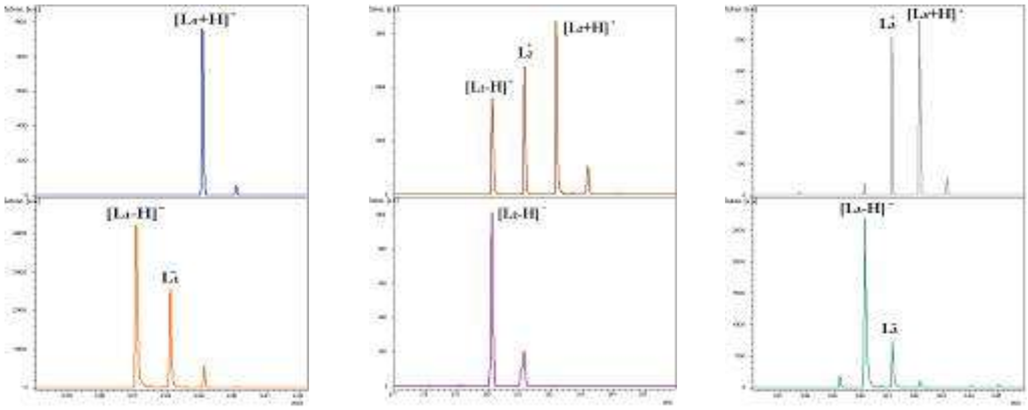

Fig. Fragments of flavonols mass spectra: *1* – L1, *2* – L2, *3* – L3; at their desorption from the standard steel substrate

Thus, the availability and the intensities of the peaks of the group of molecular ion in mass spectra of the flavonols studied correlate with the redox properties of these compounds. The presence of additional electron-donor groups in the flavonol derivatives increases percentage of oxidized forms in mass spectra.

Adsorption of lead(II) and cadmium(II) ions by mesoporous silica functionalized with diethylphosphatoethyltriethoxysilane via direct template method

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It is known that functionalized mesoporous silica adsorbs metal ions due to the complex formation. The interaction between metal ion and functional groups may be presupposed using Pearson acid base concept [1].

To determine the affinity of different metal ions to the phosphonic acid groups we carried out their sorption from water solutions. Under identical conditions at the ratio of the solid to liquid phase 1:100 the value of sorbed ions increased in the row: $Co^{2+} < Ni^{2+} < Cd^{2+} < Zn^{2+} < Cu^{2+} < Nd^{3+} = La^{3+} < Sm^{3+} < Pb^{2+} < Dy^{3+}$.

For the further investigations we chose such heavy metal ions as lead(II) and cadmium(II). Furthermore, according to the 1998 Aarhus Protocol on Heavy Metals to the United Nations Convention [2] they were considered as the most hazardous environmental pollutants.

To investigate the sorption potential of functionalized mesoporous silica we determined the amount of chemically available functional groups (1-2 mmol/g) by potentiometric titration. We calculated the sorption capacity, distribution coefficient, exchange constant, and the ratio of the groups to the sorbed ions using the adsorption isotherms of lead(II) and cadmium(II) ions.

Such parameters as the rate of saturation and regeneration ability defined the potential application of functionalized mesoporous silica as a sorbent. The data obtained from our analysis of sorption kinetics demonstrated that saturation was achieved within 5-15 minutes.

Since silica-based sorbents are environmentally friendly and thermostable, they can be used in multi-cycle sorption processes. For these reasons, functionalized mesoporous silica could be proposed as sorbents for industrial wastewaters treatment.

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Kinetics of optical response of films NiOOH in the presence of formaldehyde

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One of the dangerous carcinogenic and toxic substances which falls into a stock water is formaldehyde [1]. In this connection it is necessary to develop sensory materials for its definition in solutions. We have studied the optical properties of the films $Ni(OH)_2$ in the presence of formaldehyde. Films $Ni(OH)_2$ were obtained by the method described in article [2]. Formaldehyde is known to be inherently strong reducing agent, and nickel hydroxide, oxidized at the anode to NiOOH - oxidant. We investigated the kinetics chemichromic transformations of NiOOH films in formaldehyde solution. The change optical light transmittance, of transparent electrodes $NiOOH/SnO_2$/glass in the presence of formaldehyde was determined. From analysis of kinetic curves it was found that the area of maximum optical sensitivity NiOOH electrodes occurs within 1-11 mmol/l formaldehyde. Herewith optical light transmission varies significantly over ~ 2 min. Determination of the lower concentrations of formaldehyde requires from 5 to 10 minutes, depending on the content of formaldehyde in water. Determination of the higher concentrations of formaldehyde (22 mmol/l or more) is possible by absolute value of light transmission at the anodic polarization $E = 0.8$ V (rel. s.c.e.) $Ni(OH)_2$. Summing up studies, we can conclude that the film NiOOH can be used to determine both small and high concentrations of formaldehyde.

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Liquid-phase synthesis of $LiFePO_4$ nanocrystals and properties of obtained cathode material

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Nanocrystals $LiFePO_4$ (LFP) with olivine structure is effective cathode material for lithium-ion battery [1]. The main drawbacks of LFP are the low electronic conductivity and Li^+ diffusivity. These parameters can be improved in the formation of the crystal structure of LFP during the phase of long high-temperature annealing of amorphous synthesized $LiFePO_4$ powders [2]. However, this traditional approach has exhausted itself. This prompted us to offer a low-temperature synthesis method in salt melts. Such approach allows us to obtain nanocrystalline $LiFePO_4$ in one stage.

In order to obtain cathode composite material with optimal properties, several schemes in the liquid-phase synthesis environment were tested. We have selected fusions in which the synthesis can be realized at temperatures of 150-700 °C and observe the influence of melt components and precursors on the nature of synthesis, the structure of resulting products, and bind these parameters with physical and chemical properties of the precipitate. The LFP synthesis in nitrate and chloride systems is characterized by the presence (appearance) of oxide and phosphate admixtures together with the main phase. It is concluded that for optimal characteristics of the material we need to minimize the impact of oxidants and provide a stoichiometric ratio of precursors. In this regard, the low-temperature acetate eutectic $CH_3COOK\text{-}Cd(CH_3COO)_2$ and eutectic mixture of choline chloride and diethyleneglycol were selected. It helped to get the LFP without admixtures.

The synthesized $LiFePO_4$ powder composed of crystals with an olivine structure and size of 30-55 nm (XRD), agglomerates are visible (SEM). According to the EDX analysis, elemental composition of the resulting product refers to $LiFePO_4$. Electrodes based on synthesized LFP powders have been tested by CV method and charge/discharge characteristics. Obtained results characterize the process of Li^+ incorporating into the $LiFePO_4$ as reversible, with the value of the charging capacity of about 135 mAh/g.

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Strontium ions sorption on composite sorbent based on lignocellulose and hydrated antimony pentoxide

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Strontium is present in the environment as a decay product from nuclear power plants, and also produced in the reprocessing of nuclear fuels, such as ^{89}Sr and ^{90}Sr with half-life of 51 and 29 years respectively. Removal of radioactive strontium from liquids ensures health security and environmental protection.

For this purpose in our research work the possibility of application the composite lignocellulose-inorganic sorbents based on lignocellulose (LC) wastes of food industry modified with hydrated antimony pentoxide (HAP) was investigated. The LC-product with the content of cellulose and lignin are 28 and 66 % respectively was used through experiments. During treatment of the LC with $SbCl_5$ the hydrolysis of antimony chloride in water solution with the formation of $Sb_2O_5{\cdot}nH_2O$ and its sedimentation on the carrier bulk took place and LC-HAP sorbent is formed. Composite LC-HAP characterized by modifier content 2.8 %. The adsorption of strontium ions was determined by the radiotracer method using radioisotopes.

The removal efficiency of strontium ions from model solution and distribution coefficient on LC-HAP are 97.3 % and $1.2{\cdot}10^3$ ml/g respectively. At the same time the distribution coefficient of strontium ions on bentonite is $1.4{\cdot}10^3$ ml/g, clinoptilolite – $0.8{\cdot}10^3$ ml/g, synthetic zeolites such as erionite, NaA, NaY and NaX are $0.2{\cdot}10^3$, $0.4{\cdot}10^3$, $0.2{\cdot}10^3$ and $0.5{\cdot}10^3$ ml/g respectively. Comparing the values of the distribution coefficient of strontium ions on LC-HAP with the literature data, it is possible to argue about high effectiveness of the obtained sorbents. It is known that pure LC-materials do not show affinity for radionuclides so the values of the distribution coefficient of radionuclides can be recalculated on the mass of modifier in LC-inorganic sorbents, so the specific distribution coefficient was calculated. The value of the specific distribution coefficient of strontium ions on HAP in the bulk of LC-HAP sorbent reaches $4.3{\cdot}10^4$ ml/g.

Obtained sorbent can be used as material of multifunctional purposes: as sorbents in radiochemistry and analytical chemistry as well as in ecology and as enterosorbents in medicine and in veterinary.

Nanocomposition for wound care Pathelen®: pharmaceutical and technological aspects

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Healing of infected ulcers and wounds, particularly in old men, is of serious problem in modern surgery. Clinical practice shows that the treatment of purulo-inflammatory diseases and purulent wounds by using antimicrobial agents only, does not always lead to the desired result. Misuse of antibiotics contributes to the emergence of resistant (hospital) strains of pathogenic microorganisms, including methicillin-resistant *Staphylococcus aureus* (MRSA). The intensity of the regeneration process and healing of wounds depends largely on the speed at which they are cleared from the pus and necrotic tissues. For this purpose sorption-applique treatment, i.e., a method of wound healing in which an absorbent in powder form is applied to the wound as a powder dressing, can be used. This approach is well known in Ukraine but is practically undeveloped in the countries of EU.

We have elaborated the new composition Pathelen® based on synthetic highly disperse silicas that has high absorptive, anti-inflammatory and wound-healing abilities. The content of Pathelen® may be varied, depending on the phase of wound healing process. The basic composition contains ingredients, which are allowed for clinical use and certificated in Ukraine and in EU, namely, nanosized silica (Aerosil 300), hydrophobic silica (Aerosil R972 Pharma) or polymethylsiloxane and benzalkonium chloride. Pathelen® belongs to a group of application sorbents with antimicrobial effect.

The manufacturing of Pathelen® consists of *i*) immobilization of benzalkonium chloride on the surface of hydrophobic silica by the treatment in ball mill, and *ii*) mixing of nanosized silica with semi-product obtained in step (*i*) in the mixer with vane. The final quality control includes the IR spectroscopy examination, identification and purity tests, study the adsorption activity relatively to gelatin and control of microbial contamination. Particularly, it was shown the absence of pathogenic microorganisms and fungi, the quantity of non-pathogenic microorganisms is less than 100 units per 1 g that complies to requirements of European Pharmacopoeia to the products of this category.

Property on the composition Pathelen® is protected by European patent PCT/EP2015/075724. The applicant and owner is Invenres GmbH, Switzerland.

Self-organization of carbon nanotubes in evaporating droplets of toluene and isopropanol suspensions with presence of Triton X-165

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Particle redistributing during the drying process of colloid solutions droplets can be controlled by regulating of external chemical and physical conditions [1]. Additives of surfactants can significantly affect the processes of structure formation in suspensions of nanotubes based on organic solvents [2].

The aim was to study the influence of additives of nonionic surfactant (Triton X-165) on the patterns formation during drying of droplets of multiwalled carbon nanotubes (MWNT) suspensions in isopropanol and toluene.

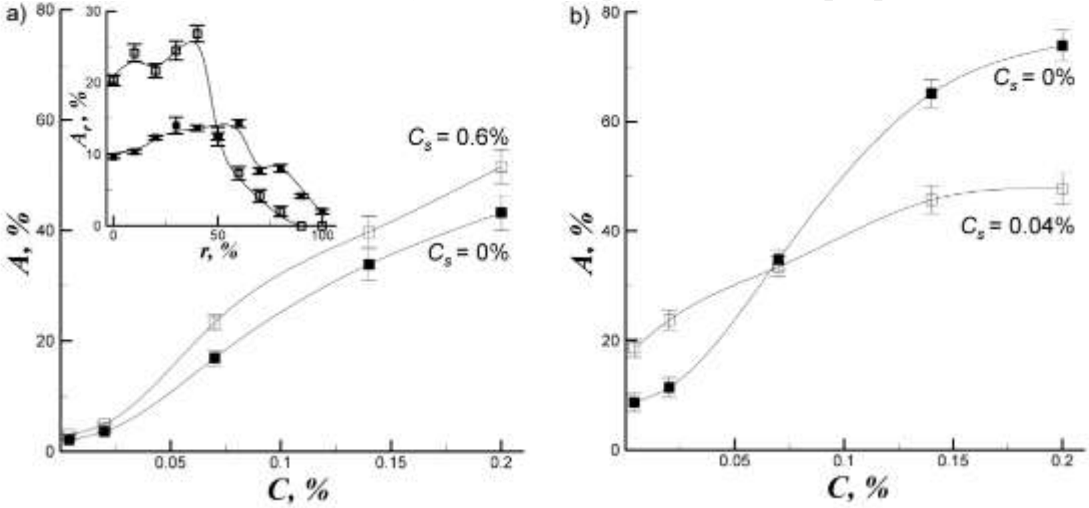

Fig. Light absorption *A* by dry patterns of MWNT obtained from droplets of toluene (*a*) and isopropanol (*b*) suspensions, for different initial MWNT concentrations, *C* and for different initial surfactants concentrations, C_s. On inset – absorption Ar on the dry film depending on the distance from the center *r* (*C*=0.02%)

Fig. shows that increasing of concentration of MWNT-based suspensions in isopropanol and toluene leads to increase of size of MWNT aggregates in final dried films. It is expressed in the growth of integral light absorption by dry patterns *A*. Surfactant additives accelerate growing of light absorption in toluene suspensions (*a*) and retard for suspensions based on isopropanol (*b*). Most of dispersed material settled near the drops center as aggregates (inset on Fig., *a*). ”Coffee ring” structures were not observed.

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Hydrated properties of initial tannin and tannin–methylsilica composite system

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The perspective direction in the creation of microfertilizers is using composite system which based on nanosilica and substance-sensitizer. Substance-sensitizers are conductors of nutritional minerals, providing high growth and increasing their resistance to different diseases. Tannin may be one from these substances

So, the aim of this work was studying of bonding initial tannin and tannin-hydrophobic methylsilica composite system with water.

^{1}H NMR spectra of initial tannin, containing 50 mg/g residual water in the air medium, shows only signal of adsorbed water (chemical shift δ_H=4.5-6 ppm). This means that the present type of bound water is strongly associated water (SAW, every molecule participates in the formation of two or more hydrogen bonds). The spectra become more complicated for water adsorbed in the composite system which prepared by mechanochemical activation of equal weight parts of tannin and methylsilica. There are clusters of strongly and weakly associated water (WAW) on the surface of composite system. The part of WAW increases with temperature decreasing.

Thus, ^{1}H NMR spectroscopic studies allows us to assume, that the stimulating effect can be observed due to the formation of a significant amount of weakly associated water in the germination zone, which will improve the mass exchange of germinating seeds with the surrounding medium.

Measurement accuracy of gelatin adsorption onto nanosilica surface

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The pharmacological activity of preparations based on nanosilica can be determined from the value of gelatin adsorption. Ten adsorption isotherms were obtained under the same conditions to determine the accuracy of measuring the maximum adsorption ($A_{\max}$) of gelatin on the surface of fumed silica (Fig.).

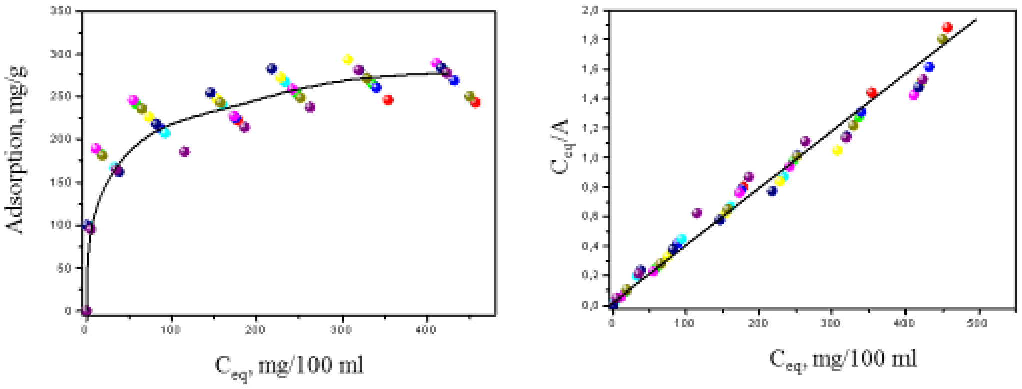

Fig. Isotherms of gelatin adsorption on the silica surface in standard (left) and linearized (right) forms

Based on the obtained isotherms, the maximum adsorption values were calculated and the measurement errors were determined (Table). As a result of the calculations, the arithmetic mean of the measured values of A_{midle}, their standard deviation s, standard deviation of the arithmetic mean s_m and the variance of the distribution s^2 were obtained.

	Initial concentration of gelatin, mg/g							$A_{\max}$, mg/g
	100	200	300	400	500	600	700	
A_{midle}	99.7	169.4	217.2	235.1	258.4	272.6	272.9	277.5
s	1.6	10.4	20.9	14.3	16.8	13.3	15.0	14.9
s^2	2.6	108.2	436.8	204.5	282.2	176.9	225	222
$s_m\,\alpha$	1.2	7.9	15.8	10.7	12.7	10.0	11.3	11.2
$A_{\text{midle}} \pm s_m\alpha$	99.7 ±1.2	169.4 ±7.9	217.2 ±15.8	235.1 ±10.7	258.4 ±12.7	272.6 ±10.0	272.9 ±11.3	277.5 ±11.2

The described technique of treatment of the protein adsorption isotherms on the silica surface makes it possible to obtain highly reproducible results.

Effect of ethonium adsorption on structure formation in nanosilica dispersions

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Gemini surfactants, including quaternary ammonium salts, are used in many industrial, agricultural and medical applications due to their unique physicochemical and biological properties [1, 2]. In the case of the surfactant adsorption onto a solid surface, the structure and properties of surfactant define the interaction with solids, as well as structure of a surface layer. The behavior of surfactants at a solid surface is determined by a number of forces including electrostatic attraction, covalent bonding, hydrogen bonding, hydrophobic bonding and solvation features [3]. Usually, ionic surfactants interact with a silica surface by electrostatic attraction between charged parts of surfactants molecules and surface hydroxyl groups.

The adsorption of gemini surfactants ethonium onto the fumed silica surface and its influence on the colloidal properties of aqueous dispersions were investigated. The adsorption isotherm corresponds to the two-step model with a pronounced plateau at ethonium concentration less than critical micellar concentration (CMC) and a marked increase in the adsorption at CMC due to the formation of hemimicell in the surface layer. The adsorption of ethonium leads to compensation of silica surface charge and changes in the shape of the pH-dependence of the zeta-potential. The increase in the particle sizes in the aqueous dispersions of silica is observed due to ethonium adsorption. The colloidal stability of the dispersions with silica concentration of 5 wt.% is improved at ethonium presence, while for 1 wt.% dispersions the ethonium almost does not affect the stability. The rheological properties of the dispersions depend on the ethonium concentration, and the maximum values of the viscosity and rheopectic behavior are observed at ethonium concentration of 0.1-0.3 wt.%.

Acknowledgements
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Investigation of chitosan-based nanocomposites with immobilized natural bactericides

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Tannins are natural antioxidants with unique properties such as hydrogen electron splitting and electron elimination, considered potential inhibitors against reactive oxygen or nitrogen species and efficient antimicrobial activity. Due to the unfavorable pharmacokinetics of conventional antioxidants, they manifest a rapid metabolism with formation of secondary metabolites and a considerable reduction in their time of action [1]. For the enhancement of its antioxidant and antibacterial properties, entrapment of natural biocides into a natural matrix can be used for prolongation of their biological activities. Biopolymers such as chitosan (CS), cellulose, dextran are supramacromolecular biocompatible compounds with low toxicity and biological recognized by the cell entities [2].

The present work was undertaken to determine the detailed morphology of the chitosan-based compositions (hydrogel, films), containing biocide Enoxil and hydroxyethyl cellulose (HEC) and glycerin (Gly) as stabilizers and enhancers, using atomic force microscopy, DSC, NMR, FT-IR and others.

The results showed that the addition of Enoxil into CS solution changed the morphology (sizes of nanodomains and roughness of the free sample surface), as well as the porosity of the bottom films surface. Moreover, DSC and DMA analysis display that the Enoxil introduction changed the thermal and relaxation properties of composite films, which can be explained via assemble at the nanolevel. Moreover, entrapment of Enoxil into chitosan/HEC/Gly matrix enhanced antioxidant capacity (AC, by 50%) as compared to Enoxil alone determined by ABTS and DPPH assays. Microbiological investigations has revealed that biomedical films chitosan/HEC – Enoxil are efficient for inhibition of growth of *P.aeruginosa* (MIC 0.1% mg/ml) and *B.cereus* (MIC 0.1% mg/ml) bacteria. Therefore, these bionanocomposites could be proposed for using in open trauma infections and as post-operative surgery.

Acknowledgements

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Nonlinear loading effects in oxide-filled polyester nanocomposites observed by IR-spectroscopy and lifetime positron spectroscopy

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Impact of nanosized oxide particles of titania (rutile) and silica-titania (STO) fumed compound on physical properties related to inner structure of a styrene-cross-linked polyester resin have been experimentally studied. The IR-spectroscopy and the positron annihilation lifetime spectroscopy were used to study the electronic polarizability of interatomic bonds and the positron annihilation processes with increasing the filler loading. All the nanocomposites show unmonotonous variations in the electronic polarization and the positron annihilation parameters. Three lifetime components, namely τ_1 with intensity I_1 which define the annihilation of quasifree positrons with great bulk electron mass of atoms forming polyester and styrene chains and components τ_2, τ_3 with and their intensities I_2, I_3 characterize annihilation of captured positron and positronium by traps of various radia R_+ and R_{ps} and the electron density on the defect walls have been determined. The lifetime concentration dependences exhibit nonmonotonous reduction in the low loading range of fillers at $C_{f,m} < 3\%$ with the minima values at $C_{f,m} = 1.5$ % for the unfilled resin and its nanocomposites. There are some distinctions between the lifetime dependences in the TiO_2- and STO-filled nanocomposites in the content range $C_{f,m} > 3$ %. For the composites with TiO_2 particles the lifetimes slow change in the filling range $3 < C_{f,m} \leq 5\%$, whereas for the STO-filled composites those exhibit smooth slight rise at the same content interval. The free-volume portion f_v (in %) in a polymer matrix droningly decreases in composites with STO-particles upon loading while in the composites with TiO_2 particles the f_v nonmonotonously increases. The parameters describing the supramolecular (cluster) structure, the macromolecular segment mobility, and the submolecular structural defects (pores) have been calculated using the fractal approach. Some correlations among loading-dependent properties and underlaying alterations in the resin's structure on submolecular, molecular, and supramolecular levels have been discussed.

Nanostructured high performance heat-resistant polymer materials

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Series of nanostructured high performance heat-resistant thermostable nanocomposites based on densely cross-linked cyanate ester resins (CER) was synthesized by *in situ* method using different nanofillers, such as epoxy- or amino-functionalized polyhedral oligomeric silsesquioxanes (epoxy-POSS or amino-POSS, respectively), amino-modified MMT, multiwalled carbon nanotubes (MWCNTs) *etc*. The effect of nanofillers on thermal stability and structure-property relationships of the nanocomposites created was investigated using TGA, DSC, DMTA, TEM, SEM methods, FTIR spectroscopy *etc*. The high performance nanomaterials produced can be used as thermostable adhesives, coatings and sealing compounds in airspace industry, microelectronics *etc.*

The results obtained provide a self-consistent picture of changes in the thermal stability (TGA), nanostructure and morphology (TEM, SEM), glass transition characteristics (DMTA, DSC), and chemical structure (FTIR) of the studied nanomaterials caused by introducing and chemical embedding of all the functionalized nanofillers used. Significant increasing of glass transition temperature value (by 30 - 40°, T_g ~ 270 - 290°C) has been reached by using ultra-low (<<1 wt.%) contents of amino-modified MMT resulted simultaneously in some suppression of vibrational dynamics of rings in the CER network, twofold rise of storage modulus (E'), and enhancing thermal stability ($T_{d(onset)}$ ~ 433 - 440 °C) of the CER/amino-MMT nanocomposites [1]. It has been established that the CER/MWCNTs, CER/epoxy-POSS and CER/amino-POSS nanocomposites possess improved complex of physical-chemical properties, *i.e.* higher stability to thermal-oxidative destruction, higher conductivity (for CER/MWCNTs samples), higher glass transition temperature T_g and storage modulus E' values compared to unfilled CER.

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Enzyme mimetic activity of kaolin clay supported nanoceria

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Nowadays enzyme mimetic activity of synthetic materials that can perform the functions of natural enzymes is widely investigated and studied. In this respect cerium oxide nanoparticles shows excellent prospects because of due to the unique structure demonstrate similar properties to the two key antioxidant enzymes, catalase and superoxide dismutase, which react catalytically with superoxide and hydrogen peroxide. The aim of this work is the preparation of new nanomaterials by modifying of kaolin clay by nanoscale cerium oxide, the identification of physical and chemical properties of synthesized nanocomposites, experimental determination and comparison it's enzyme mimetic activity in a model reaction of hydrogen peroxide decomposition at different pH of reaction medium.

A series of kaolin nanomaterials decorated with CeO_2 were synthesized by reaction of cerium nitrate deposition in an aqueous medium without stabilizers at room temperature. Nanocomposites were characterized by SEM and TEM. The size of CeO_2 nanocrystals ranging from 5.6 to 10.4 nm and amounts of deposited cerium oxide in nanomaterial vary from 2.76 till 7.37 % as shown by atomic emission spectrometry analysis. X–ray analysis of samples shown that deposited cerium dioxide has a cubic structure. $I_{\mathrm{UVSCe}}{}^{4+}/I_{\mathrm{UVSCe}}{}^{3+}$ ratios in nanocomposites were evaluated by UV diffuse reflection spectroscopy. The catalytic activity of the synthesized materials, kaolin, and pure cerium nanooxide was investigated in a reaction of H_2O_2 decomposition in pH range 8.5 – 10.5 and compared with the enzyme catalase activity. Volumetric method was used to determine the kinetic of hydrogen peroxide decomposition. Michaelis constants (K_m, mM) were applied for analysis, quantitative assessment and comparison of enzyme mimetic activity of nanomaterials and enzyme catalase.

The dependence of the nanocomposites activity on pH is extreme with maximum at pH 9.5–10. We suggested a linear dependence of the catalytic activity of the material from CeO_2 content in nanocomposite. Catalase mimetic activity of studied materials in terms of 100 % content of cerium oxide CeO_2 correlate with nanooxide particle dispersion and ceria surface defects, evaluated as $I_{\mathrm{UVSCe}}{}^{4+}/I_{\mathrm{UVSCe}}{}^{3+}$ ratio.

Nucleophilic addition of macrocyclic amines to fullerene C_{60}

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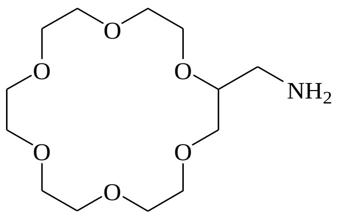
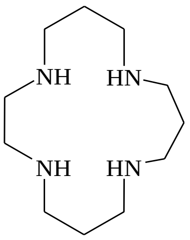
Nucleophilic addition of amines is a convenient reaction for incorporation of diverse organic groups into fullerene cage. The goal of the present work was to test the possibility of covalent attachment to C_{60} of two macrocyclic compunds: 2-aminomethyl-18-crown-6 (hereafter AM18C6) and 1,4,8,12-tetraazacyclopentadecane (TACPD) under solvent-free melting conditions. The reactions were performed at *ca*. 160 °C for 5 h in vials sealed under vacuum. The nucleophilic addition of the macrocyclic compounds under the study most likely takes place at the 6,6 bonds of pyracylene units, as in the case of other amines. The products of AM18C6 and TACPD reaction with C_{60} were characterized by means of scanning electron microscopy, Fourier-transform infrared and Raman spectroscopy, thermogravimetric analysis, as well as laser desorption/ionization time-of-flight mass spectrometry.



AM18C6



TACPD

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Carbon nanomaterials as catalysts in lauroyl peroxide decomposition

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Disposal of organic peroxides is an extremely urgent problem. Catalytic decomposition of organic peroxides can be proposed as an effective method to solve this problem. Carbon nanomaterials (CNM) such as activated carbon (AC), carbon nanotubes (CNT) are extensively used as catalysts for organic and inorganic processes. In this study, the catalytic activity of CNM in the model reaction of lauroyl peroxide (LP) decomposition has been investigated and compared with catalytic activity of natural enzyme catalase.

A number of carbon based materials such as natural (KAU) and synthetic (SKN) AC and CNT, their modified forms – oxidized: SKN_O, KAU_O, CNT_O; nitrogen containing (KAU+N, KAU_O+N, N-SKN, N-KAU, N-CNT, KAU_O-NH_2) and catalase (from bovine liver, Fluka) have been used as catalysts in reaction of LP decomposition. The investigated samples were characterized: specific surface area and average pore radius – by argon low-temperature adsorption-desorption method; sorption pore volume – by desiccator method, elements composition by Prehlya and Dumas methods. The chemical state of nitrogen on the surface of samples has investigated by X–ray photoelectron spectroscopy; qualitative and quantitative characterization of functional groups on the surface - by Böhm titration. Michaelis constant (K_M, mM) and reversed to it affinity constant (K_{af}, mmol^{-1}) have been used to calculation of CNM and their modified forms catalytic activity from kinetic data.

It has been found that the catalytic activity (K_{af}) of the investigated materials in reaction of LP decomposition decreased in the following order: N-KAU (30.3) > N-CNT (21.3) > N-SKN (11.1) > SKN (6.2) > SKN_O (5.3) > KAU_O-NH_2 (4.9) > CNT (4.4) > catalase (4.3) > KAU (3.8) > CNT_O (3.6) > KAU_O+N (3.4) > KAU_O (3.1) > KAU+N (1.8). The highest activity (higher than catalase) exhibit nitrogen-containing CNM (N-KAU, N-CNT, N-SKN). Functionalization of carbon nanomaterials by oxygen and nitrogen changes electrondonating ability of CNM surface, leading respectively to decrease or increase of their catalytic activity in the reaction of LP decomposition. It is found that the catalytic activity of studied samples correlated with surface basicity and presence of quaternary nitrogen groups in structure. Therefore, nitrogen-containing materials N-KAU and N-CNT can be used as efficient catalysts for the organic peroxides decomposition.

Optimization of size of periodic structures for solar cells

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In recent decades, world solar energy is developing at a high rate, solar power plants are becoming part of the energy infrastructure of many countries. The development of solar technology has a significant impact on the economy. It can be expected that in the coming decades solar energy will become a stimulus for the economic development of countries and regions that have the maximum solar resource.

When periodic silicon structures are used as solar cells, it is known that their efficiency depends on the size and the period of such structures. Our task is to optimize the size and frequency of microstructures depending on the heat sunlight. It is known that an increase in temperature of solar cell efficiency is reduced because there is a need to optimize to this parameter.

For theoretical calculations used silicon periodic structure with the following parameters: the thickness of the substrate - 5000 nm, the column height - 2000 nm, periodicity (*P*) - 300-1200 nm the ambient temperature - 25 ^{o}C, the intensity of solar radiation - 1000 W/m^2, $D/P = 0.8$, *D* - diameter of columns.

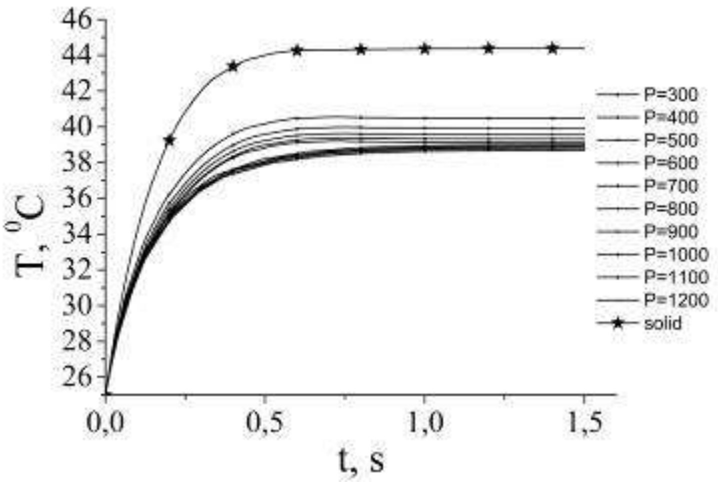

Fig. Dependence heating temperature structure over time for different values of period structures

It is shown (Fig.) that the periodic structure is heated less than solid silicon plate. Increasing the period of structure leads to a reduction of temperature heating.

Concept of nearest neighborhood at the percolation model of surface defects

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Theoretical and applied percolation studies conducted in the beginning of the century once more shown interesting results of various authors on the effect of properties and features of the evolution of connected and quasi-connected areas on surface of materials on its structure and functionality, and provoked development of adequate mathematical tools for the description of critical phenomena.

In the report concept is offered of the nearest neighborhood of structural elements of surface defect's clusters. Such concept allows formulating special percolation model of system defects. Dominant trait of that model is all-out multiscales of structure elements, which significantly extend capabilities of theoretical studies of defect's clusters generation and their properties [1, 2].

In presented model, the nearest neighborhood of elements of the cluster system is percolation fields that are located around it in the phase spaces of the properties.

One of important the model's aspect is to consider the nearest neighborhood like set belonging to the class of "thick" fractals. The report described the algorithm for determining the Lebesque measure on the set of "conductive" sites of the nearest neighborhood and the algorithm for calculating the dimension of describing the scaling behavior of their division’s entropy. In addition, the set-theoretic description of percolation transitions in the continuum and fractal structures is given; the idea of the relative degree’s order of the structure is introduced, and justification of it's for suitability to evaluate the drift of the nearest neighborhood properties is presented.

Thus defined the immediate neighborhood and the complex components create, in fact, a new type of multidimensional phase spaces for percolation problems. This will allow almost arbitrarily increase the number of parameters of which depend on the characteristics of percolation clusters, which in turn may lead to new classes of percolation problems and new applications. The report also provides the physical substantiations of the proposed model.

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Dynamic mechanical analyses and thermodynamics of POSS-containing nanocomposites based on PU/PHPMA semi-IPNs

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The impact of different amount of the 1,2-propandiolisobutyl-POSS (1-10 wt%) on the dynamic mechanical behaviour and thermodynamic miscibility of nanocomposites based on semi-interpenetrating polymer networks (semi-IPNs) of the crosslinked polyurethane (PU) and linear poly(hydroxypropyl methacrylate) (PHPMA) have been investigated.

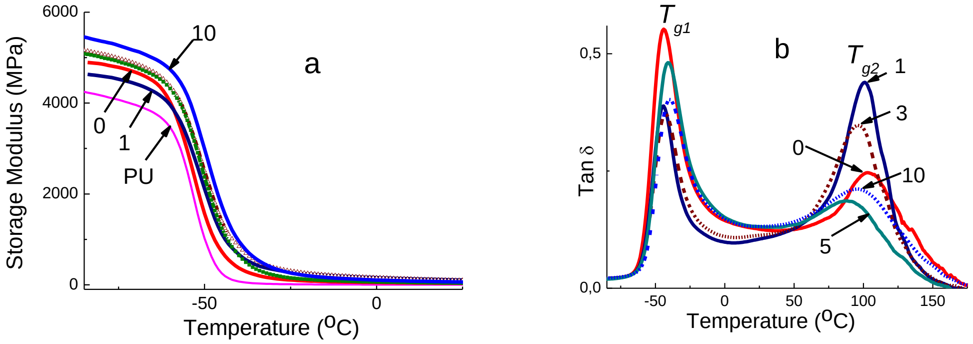

Fig. Temperature dependences of the storage modulus (*E*') and the loss factor (tan *δ*) of semi-IPN-based nanocomposites with different POSS content (0, 1, 3, 5, 10 wt.%)

The DMA results of POSS-containing nanocomposites are compared with that of native PU/PHPMA=85/15 semi-IPN and PU (Fig.). As clearly seen from Fig., *a*, the storage modulus (*E*') of the nanocomposites increases with increasing of POSS content. Fig., *b* shows that all nanocomposites based on semi-IPNs are two-phase systems with incomplete phase separation.The glass transition temperature T_{g1} (peak Tanδ) of PU shifted towards higher temperatures with increasing the POSS content, but T_{g2} of the second component (PHPMA) in the semi-IPNs is shifted downward. The redistribution of Tan δ peak amplitudes depends on the composition and evidences of the formation more or less interfacial area between two polymer components (PU and PHPMA). The introducing of small POSS amount (1-3 wt.%) leads to increasing of the phase separation in the nanocomposites, but further growth of POSS content (5-10 wt.%) results in lowering the phase separation, perhaps due to formation of the POSS clusters which physically connected with both polymer components. The thermodynamic parameters of the interactions in the POSS-containing nanocomposites were calculated and they are in accordance with α-degree of the phase segregations of components.

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The structure, morphology and optical properties of nanostructured NiO thin films deposited by magnetron sputtering at diverse conditions

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NiO is a wide-gap direct band gap *p*-type semiconductor material (E_g=3.5–4.0 eV at room temperature). Due to its low cost, electrochemical stability and a great durability as well as unique optical, electrical and magnetic properties, NiO is considered as an attractive material for development of *p*-type transparent conductive films, ultraviolet detectors, solar cells, spin-valve giant magnetoresistive sensor, electrochromic window devices, gas sensors, *etc*.

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 easy control over the composition of the deposited films. It is obviously that the enhancement both crystal quality of NiO films and their optical and electrical properties can be reached by the optimization of film growth parameters. The layer-by-layer growth method in magnetron sputtering was early proposed by us for improvement of ZnO films crystalline structure [1].

Therefore, our report is devoted to investigation of the influence of such technological parameters of MS as substrate temperature, oxygen and argon pressures, magnetron power and substrate bias on structure, morphology and optical properties of NiO thin films deposited on Si (111) and glass substrates by layer-by-layer growth method at MS. The properties of NiO films were studied by X-ray diffraction, atomic force microscopy, energy dispersive X-ray spectroscopy, Fourier transform infrared spectrometry and optical transmission measurements. Obtained results will be discussed and presented.

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.

The investigation of highly-doped ZnO:Al,N films grown at oxygen-rich conditions

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ZnO has been intensively investigated as a promising material for development of effective optoelectronic devices because of its wide-band gap of 3.3 eV and large exciton binding energy (60 meV) at room temperature. An investigation of the highly-doped ZnO:Al,N films is attractive for obtaining *p*-type conductivity in ZnO as well as for an improvement of performance of ZnO-based ultraviolet detectors.

Highly-doped ZnO:Al,N films were grown under oxygen-rich conditions on Si substrates by magnetron sputtering using a layer-by-layer growth technique [1]. X-ray diffraction, scanning electron microscopy, energy dispersive X-ray analysis, X-ray photoelectron spectroscopy, X-ray emission spectroscopy and secondary ion mass spectrometry were used for the samples characterization. It was shown that nitrogen in ZnO has a solubility limit when a phase of zinc nitride is formed in ZnO lattice. The X-ray photoelectron spectroscopy demonstrates that nitrogen has different chemical bonds that depend on the deposition parameters. With increasing of nitrogen content the position of Fermi level for ZnO:Al,N is shifted in conduction band, thereby causing the electronic conductivity in the films. The reasons of such behaviour of conductivity are discussed. An effect of high aluminum and nitrogen doping on structure and electronic properties of ZnO films was studied and discussed.

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Synthesis, optical and photocatalytic properties of nonporous platinum-doped titania films

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Semiconductor photocatalysis is widely studied in recent years for application in environment purification [1]. Most photocatalysts are, however, wide band-gap semiconductors which are active only under UV irradiation. In order to effectively utilize visible solar radiation, the investigations of various types of visible-light active photocatalysts including metal ion-doped TiO_2 nanocomposites is investigated. Numerous metal ions, including transition metal ions (e.g., vanadium, chromium, iron, nickel, cobalt, ruthenium and platinum), are investigated as potential dopants for visible-light induced photocatalysis. However, metal ion dopant can also serve as a recombination center, resulting in decreased photocatalytic activities. Still the key points in photocatalysis are remained the design of synthesis procedure and conditions of photocatalyst treatment to obtain the active nanocomposites under solar light.

Platinum ion-doped TiO_2 and bare titania films were synthesized using sol-gel method. Platinum(II) acetylacetonate was previously dissolved in acetone and, then, titanium isopropoxide was added to the acidify mixture. After 10 min stirring, the sol was ready for “dip-coating“ procedure. The “fresh” films were obtained onto the previously cleaned by soap and dried at less than 90 °C with the withdrawal speed of 1.5 mm/s. The one-layered and three layered films were calcined at 450 °C with heating rate was 7 °C/min. This simple and chip synthesis procedure allows to obtain nonporous active photoactive films [2]

The absorption spectra of bare titania and Pt-doped titania revealed that the band edge of Pt/TiO_2 absorption spectrum is shifted to the higher wavelength in compare to TiO_2 one. This can point on the narrowing of band gap of doped semiconductors.

Photocatalytic activity of the films was tested in the toxic dichromate ions reduction. The Pt–doped samples showed the enhancement in photocatalytic activity under UV and visible irradiation comparing with pure titania films. The most active film was 0.1 % Pt/TiO_2 one layered films.

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Formation of antibacterial coatings on chitosan matrices by magnetron sputtering

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Biodegradable chitosan matrices are used as a material for biomedical devices, implants, scaffolds. Copper coatings and nanopowders have bacteriostatic and bactericidal properties.

The purpose of our work was to obtain copper coatings on chitosan matrices by magnetron sputtering, to select the optimum sputtering regime, to study the physicochemical and antibacterial properties of the material. As chitosan matrices, chitosan films were used. The films were obtained by casting the 2% solution of chitosan in 1% acetic acid on a teflon substrate (resulting film thickness 0.03-0.3 mm).

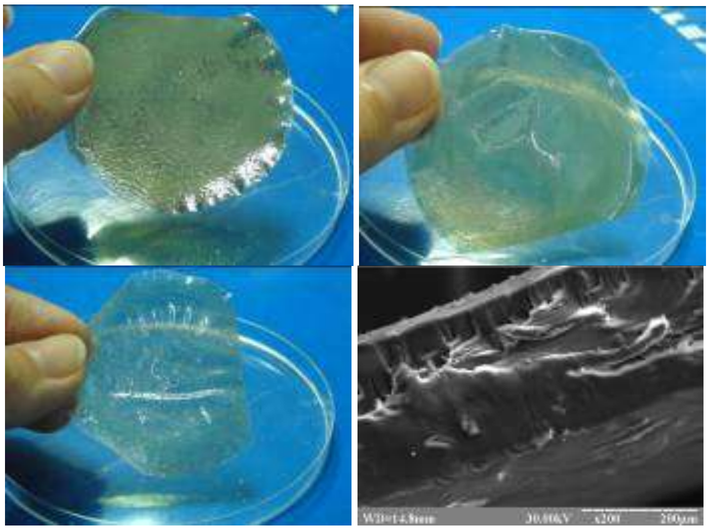

Fig. Chitosan films with different types of copper coatings and electron microscopy of the film’s cross section (right below)

As a result, modified chitosan matrices were obtained. Copper sputtering does not significantly affect the complex of their physicochemical properties, but imparts antibacterial properties; in particular, the films suppress the *St. aureus* growth.

Structural factors of crown ethers interaction with aerosil surface

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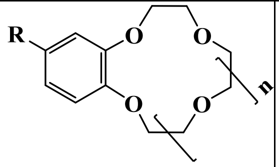
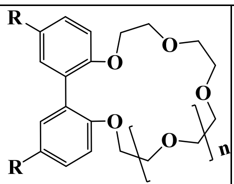
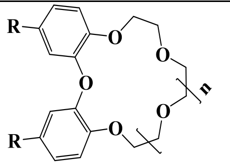
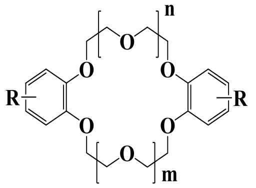
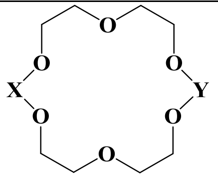
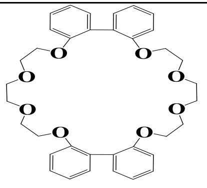
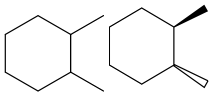
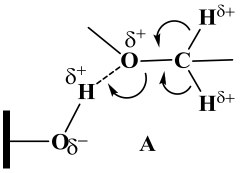
Attempt to consider the influence of structure and composition of benzo- (BCE), dibenzo- (DBCE) and "aliphatic" crown ethers (more than 40 CE) on the peculiarity of their interaction with the surface groups of Aerosil A-300 (AS) by comparing Henry coefficients (K_H) and Langmuir constants (K_L) was made.

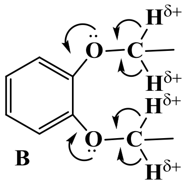
			
			R=H, *t*-Bu, NH_2, CHO, NO_2 *n*=0,1,2,3; *m*=1,2,3; X,Y= C_2H_4 and 

Three series of CE (N=10, 18 and 11)were found. In each of them the close ($0.99 \geq R^2 \geq 0.97$) dependences $K_H = a_m K_L + b$ are realized and the summand b is authentically different from zero. Similarly to the K_H [1], between the constants K_L and the desorption degrees (d) of BCE and DBCE a power-law is observed and in this case two "families" ($K_L \cdot 10^{-4} = 33 \cdot d^{-1.5}$ and $K_L \cdot 10^{-4} = 39 \cdot d^{-1.2}$) are clearly distinguished.

QSPR (Quantitative structure-property relationships) analysis [2] of the CE’s structure influence on the K_H showed the adequacy of resulting model and the greatest influence by electronic polarizability (EP, 33%) and electrostatics (ES, 29%) and, to a lesser extent, the lipophilicity (LP, 17%) and the nature of atoms (NA, 14%). Similar calculations for K_L constants show that the most influence are rendered the NA (52%) and EP (39%) while the contribution of ES is only 9%.



A



B

In the framework of the simplex approach [2], it was found that in all cases the H-atoms of the H_2C-groups promote the interaction (A) with the AS surface. Even if the O_{Ar} atoms are part of the BCE or DBCE structure "inhibiting" sorption, the polarization of the C-H bond is quite expected (B) due to the conjugation of O_{Ar} atoms with the benzene ring.

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Influence of polymeric matrix structure on physicochemical properties of composites based on TEOS

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Successfully combining the organic and inorganic components of the system, their ratio and the conditions for carrying out the synthesis, one can "combine" the properties of the individual components in the obtained polymer-silica composites, improving their performance characteristics and getting new, unique properties.

A comparative analysis of the thermal, thermomechanical, deformation properties and structural-molecular parameters of the obtained polymer-silica composites based on monomers of different structures was carried out. Nanocomposites were obtained by the simultaneous co-polymerization of mixtures of liquid organic and inorganic components. The initial compositions were prepared by mixing the sol-system TEOS:H_2O:C_2H_5OH:H_3PO_4 with monomethacrylate (HEMA) and dimethacrylate (MGF-9) at a ratio of TEOS:HEMA/MGF-9 2.5:97.5; 5:95; 10:90; 20:80; 30:70, 40:60 (vol. %).

It has been established that the physicochemical properties of organic-inorganic composites based on HEMA or MGF-9 depend on the structure of the organic matrix. Thus, for the linear polymer HEMA, a linear dependence of the increase in heat resistance and microhardness of composites on TEOS content till the microheterogenization of the structure is observed at an amount of inorganic phase ≥ 20 vol. %. For spatially cross-linked MGF-9, the influence of TEOS is nonlinear, and the composites with TEOS content 2.5 and 10 vol. % show high thermal and thermomechanical properties. In the first case, the structure in which the inorganic component in the form of nanoparticles is embedded into the polymer matrix network in microareas with a lower density, is formed, which leads to a reduction of structure defectiveness. At the introduction of TEOS in an amount of 10 vol. %, the formation of spatially cross-linked network of the inorganic component occurs, that is, the so-called interpenetrating structure ("net-to-net") is realized, which is characterized by a high level of system ordering. This organization of the structure of the obtained composites leads to improved physicochemical properties of the system.

The obtained results showed that the thermal and thermomechanical stability and microhardness of TEOS-polymer organic-inorganic composites is a complex function of the chemical nature and spatial structure of the system, which is strongly influenced by the structure factor of the introduced organic component.

Properties of model systems based on nanosilica for water bioremediation

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Nowadays, purification of the environment from the pollutants originated in petroleum production becomes very topical. To solve this problem, the bioremediation way based on the processes of petroleum products decomposition by means of microorganisms that are able to oxidize hydrocarbons is the most perspective method. The model composite system based on the mixture of nanosilicas powders and *Saccharomyces cerevisiae* yeast cells was created by us to destruct the petroleum products. Therefore, the aim of this research was to improve the composition of the composite by adding the mineral compounds that can increase the efficiency of yeast cells in the destruction of motor oil hydrocarbons and to investigate the pH influence of aqueous media on the bioremediation.

It was found that the presence of the mixture of hydrophilic (A-300) and hydrophobic (AM1-300) silicas nanopowders promotes the activation processes of cell vital activity without nutrient medium. When the additional source of mineral nutrition (KCl, $CuSO_4$, $ZnSO_4$, $(NH_2)_2CO$, $Ca(H_2PO_4)_2$) is added to the nanocomposite, the increase of yeast gas evolution in 1.4 and 1.2 times as well as the biomass growth from 1.7 to 3.3 times compared to the blank; and from 1.3 to 2 times compared to the mixture of nanosilicas powders without additives was observed. The release of carbon dioxide gas by cells suspension at pH 4.0 was decreased in 2 times and raised in 1.5 - 2 times at pH 8.0 compared to the blank. Moreover, gas evolution in the alkaline medium was in 3.5 times higher than in the acidic one. It was noted that destruction of motor oil hydrocarbons can be visually observed as gradual destruction of the oil layer on the water surface (Fig.).

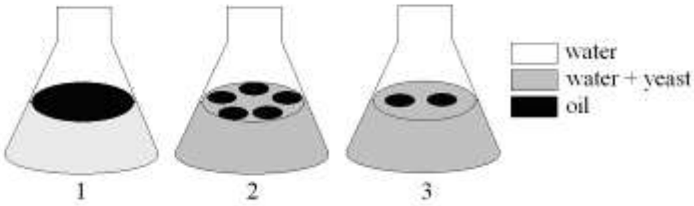

Fig. Schematic illustration of motor oil hydrocarbons destruction by the yeast cells in an aqueous media for 63 days: *1* – blank; *2* – mixture of nanosilicas powders; *3* – mixture of nanosilicas powders with mineral compounds

The experimental results obtained during this research are crucial for the development of new effective methods of water and soil purification from the motor oil pollutants.

Bulk and surface properties of binary mixtures of surfactants

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The aim of this study was to investigate the behavior of the mixtures of different types of micelle-forming surfactants and to figure out the relationship between the surface and bulk properties of the mixtures depending on the content and chemical structure of the surfactants.

Hexadecylpyridinium bromide (HDPB) and Triton X-100 were used as cationic surfactant (CSAC) and nonionic surfactant (NSAC), respectively. The mixtures of surfactants were prepared by mixing of solutions of the individual surfactants of the same concentration. Molar fraction of Triton X-100 in the mixtures was 0.3; 0.5 and 0.7.

The surface tension of surfactant solutions and their mixtures were determined by the Wilhelmy plate method. Main colloidal-chemical properties of surfactants such as maximal adsorption, surface activity and critical micelle concentration (CMC) were calculated using the surface tension isotherms. The synergistic effect, which is manifested in the reduction of surface tension and CMC, was found for the surfactants mixtures with Triton X-100 molar fraction equal to α =0.5 and 0.7. The synergistic effect was not detected when Triton X-100 molar fraction in the solution was α=0.3, while a minimal synergistic effect at low concentrations of surfactant was observed at α =0.5.

Using the Ruben and Rosen approach, composition of mixed micelles and adsorption layers at the solution–air interface, as well as the parameters of intermolecular interaction in the mixed micelles (β^m) and adsorption layers (β^σ) were calculated. These data show a degree of deviation of the mixed system from the ideal behaviour.

Comparison of quantitative characteristics of micellation and adsorption for the used mixtures of the surfactants showed the effects of negative deviation from ideal behavior during formation both of mixed micelles and mixed adsorption layers were found. The values of the interaction parameters are negative, indicating the increased attraction of molecules and ions of the mixtures in the mixed micelles and adsorption layers.

The calculations showed that HDPB/Triton X-100 micelles contain more Triton X-100 at all its molar fractions in the solution, while Triton X-100 content in the adsorption layer is higher at α =0.5 and 0.7. This is due to the higher surface activity of NSAC compared with CSAC. The molar fraction of Triton X-100 in the adsorption layer increases with an increase of its molar fraction in the solution.

Photocatalytic membranes modified with TiO_2 nanoparticles

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The preparation of membranes with photocatalytic activity is a promising area of membranology, since such membranes have antifouling and self-cleaning properties, preventing their biological and chemical contamination during filtration processes.

The industrial polyethersulfone membranes UF-PES-020H (Microdyn Nadir, Germany) with cut-off 20 kDa were used for modification. A layer of negatively charged TiO_2 nanoparticles was deposited by “layer-by-layer” method.

Photocatalytic activity of membranes modified with TiO_2 was evaluated in oxidation of Rhodamine G. The kinetic curves of the dye decomposition are shown in Fig.

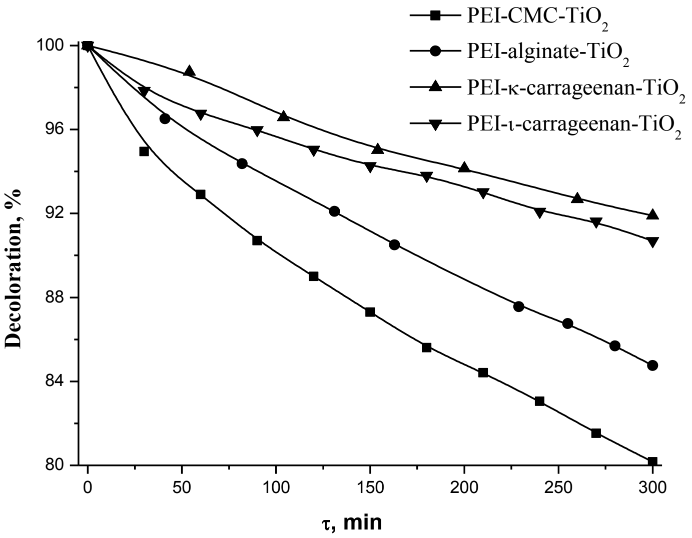

Fig. Decomposition of Rhodamine G on membranes, modified with polyelectrolyte layers and TiO_2 nanoparticles under UV light irradiation: wavelength – 300 nm; the dye initial concentration – 10 mg/L; membrane area - $2 \cdot 10^{-4}$ m^2

Experimental data show that the degradation of Rhodamine G occurs at the reaction of a pseudo-first order, and the time of half-decomposition is only 17-40 h. Such a low activity is caused by a small amount of TiO_2 nanoparticles absorbed on the membrane surface. However, it solves the problem of polymer membrane destruction during filtration and provides antifouling properties, which was proved during protein and milk filtration.

Electrochemical characteristics of $LiNi_{0.5}Mn_{1.5}O_4$ in a wide potential range

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It has been shown earlier [1] that electrodes consisting of nanosized $LiNi_{0.5}Mn_{1.5}O_4$ could be reversibly discharged during 50 cycles in the range of potentials of 2.25-3.5 V. Continuing these studies, we decided to determine the peculiarities of overlithiation (overdischarge) of $LiNi_{0.5}Mn_{1.5}O_4$ [2], a spinel cathode material for lithium ion batteries, and to study the effects of overdischarge on the further electrochemical behaviour of $LiNi_{0.5}Mn_{1.5}O_4$ in the potential range 4.9-3.5 V. Practically, long-term charging/discharging of cathodes within a wide potential range allows to examine the influence of repeated discharge on their working stability.

Upon cycling within the wide potential range including overdischarge to 2.3 V, the full initial capacity of the electrode reaches 208 mA·h/g and gradually decreases to 135 mA·h/g. R_{DC} measurements demonstrate a growth in resistance from 64 to 883 Ohm. Data obtained within the same potential range by means of CV regime reveals a decrease in intensities and a shift of peak maxima. This reflects the growth in resistance and electrode polarization. It is possible that fresh parts of the surface are formed upon the transition of $LiNi_{0.5}Mn_{1.5}O_4$ from cubic to tetragonal phase at 3 V and the thick layer of the solid electrolyte interface grows, therefore increasing the resistance of the cathode. This means that the capacity decrease arises from the kinetics of the process and is not related to the degradation of the cathode material.

Conclusions: Studies of the influence of the overdischarge (overlithiation) on electrochemical parameters of nanosized $LiNi_{0.5}Mn_{1.5}O_4$ were performed. It was determined that the overdischarge of the cathode made of nanosized $LiNi_{0.5}Mn_{1.5}O_4$ to 2.3 V leads to gradual decrease in capacity caused by the growth of resistance. Apparently, nanosized $LiNi_{0.5}Mn_{1.5}O_4$ is more affected by the growth of resistance than the microsized spinel due to the ease of formation of the solid electrolyte interface.

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New ellipsometric technique for characterization of ultrathin thermo-responsive coatings in liquid ambient

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In the last years a trend of modification of surfaces by stimuli-responsive polymers has been developed. Stimuli-responsive ‘smart’ polymers are able to change physicochemical properties upon external factor, such as temperature, pH, light, *etc*. Among diversities of the responsive polymers, temperature-responsive grafted polymer brushes deserve special attention.

Ellipsometry is a valuable tool for studying ultrathin films. It can record real-time dynamics of a film during changes in temperature or in surrounding liquid. It is sensitive to sub-nanometer changes in film thickness [1].

Molecular films are often single layers. They can be porous with a significant volume fraction containing ambient. The ambient interface can be ill defined, and surface coverage can be incomplete. Such films are called *ultrathin* to distinguish them from thicker films, which have a different optical behavior. Ultrathin films have a thickness $d \ll \lambda / 2\pi n_f$, typically < 15 nm. Since Δ is the main parameter that varies for ultrathin films by traditional ellipsometric measurement procedure, the two unknowns, d and n_f, are strongly correlated. One of possible way to overcome the correlation problem was proposed in our earlier work [2]. Measurement at the invariant Ψ-parameter in the region of low optical contrast between the transparent film and sudstrate are the main peculiarities that differ the technique suggested.

Existence the surface transition layer, which is caused by surface roughness of the substrate, is a factor that allows carrying out effective and high-precision single wavelength ellipsomertric measurements for the system of “transparent film on transparent substrate” films can be formed from polymers, proteins and amino-acids, which are intensively investigated in the last decade.

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Mesoporous ruthenium-doped semiconductive films: synthesis, optical and photocatalytic properties

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Semiconductor photocatalysis is received great attention during last three decades as a promising way for both energy generation and environmental problems. In recent years, scientific interest in heterogeneous photocatalysis has been also focused on environmental applications such as water treatment and air purification. The design and development of photocatalysts based on titania allowing their use under visible-light irradiation are under investigation. Some approaches are known, as the doping with *d*-block metals and/or non-metals as well as the dye sensitization mechanism. In the present investigation, we carry out the investigations of the effect of Ru dopant level in TiO_2 structure on optical and photocatalytic activity in the dichromate ions reduction under UV and visible light.

Mesoporous ruthenium ion-doped TiO_2 and bare titania films are synthesized using sol-gel method. Titanium tetraisopropoxide, unhydrous ruthenium chloride, a three-block copolymer of Pluronic P123 as a template in alcoholic medium and acetylacetone as a stabilizing agent were used. One and three-layered films were deposited by dip-coating procedure at a withdrawal rate 1.5 mm/s allowing the uniform covering of the film onto the glass substrate with a certain thickness. Every layer was dried at 100 °C for 30 min. The films were treated in air at 450 °C for 1 h with the heating rate of 3 °C/min. The 1, 5 and 10 mol. % of ruthenium ions in titania matrix were obtained.

The absorption spectra of bare and Ru-doped titania showed the shift of the absorption band edge towards higher wavelength for doped samples. As expected, the increase in ruthenium content leads to the higher absorption in the visible part for both one- and three-layered films.

Photocatalytic activity of the films was tested in the toxic dichromate ions reduction. The increase in the photocatalytic activity was observed for 5% Ru-doped TiO_2 films under UV and visible irradiation comparing with pure titania films. It must be noted that the adsorption of dichromate ions onto Ru-doped samples was very low.

Hybrid antibacterial nanocomposites based on silica

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Nanocomposites with biological activity is gaining a big interest in the field of nanomedicine as this capacity plays crucial role in beneficial or adverse effects of a drug or working substance on living matter [1]. Implementation of nanocomposites matrix to a drug can not only reinforce biological activity of a drug but also extend its properties [2]. For this reason, we suppose nanocomposites based on fumed silica to posses both antibacterial and healing properties against suppurative-septic processes.

The purpose of this work is to elaborate modification of commercial aerosil with specific surface area of 300 m^2/g and investigate properties of nanocomposites against *S. aureus* ATCC 25923. The modification of aerosil particles was held in the water medium with addition of commercial antibacterial drug under constant stirring at room temperature. The antibacterial activity of synthesised aerosil nanocomposites were investigated with concentrations of 1, 0.1, 0.01 and 0.001%. It was introduced that even during short (60 min) contact time with *S. aureus* ATCC 25923, the number of living cells decreased up to 98.7% and during 120 min contact – up to 99%, comparing with the control group.

Based on derived results, we may conclude that synthesised hybrid nanocomposites might be offered for treatment of suppurative-septic processes that occur in wounds. Due to great biocompatibility and ability to increase thixotropic properties of substances [3], aerosil is promising matrix for further creation of bioactive hybrid composites.

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Enoxil release from composites with silicas and polymer films

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Recently, plant polyphenols have attracted great interest as a potential antioxidant biomaterial [1]. The aim of this work was to obtain the Silica-Enoxil nanocomposites, prepare the Enoxil-polymer films and to study the active substance release rate in these systems. Silica-containing composites have been prepared by impregnation of fumed silica with Enoxil and by sol-gel silica formation into the Enoxil solution. Two or three-component films were prepared by radical polymerization of HEMA in media of copolymer solution (gelatin, vinyl acetate, chitosan). The content of Enoxil in the silica composites and polymer films was 20 wt.%.

In vitro Enoxil release test has been performed according to the requirements of the State Pharmacopoeia of Ukraine using the rotating basket method. The water has been used as a dissolution medium. The release experiment was carried out at 37 ^{o}C under stirring rate of 100 r/min. The Enoxil concentrations in released fluid were registered spectrophotometrically (at 310 nm) [2]. Typical kinetic curves of Enoxil release are represented in Fig. 1 (composites with silicas) and Fig. 2 (polymer films).

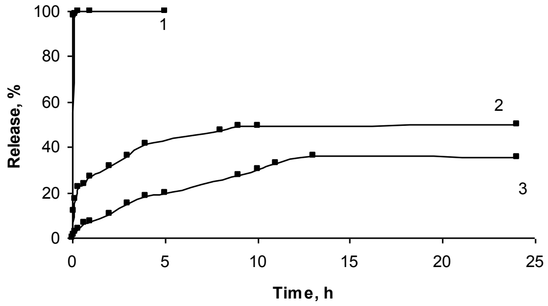

Fig. 1. Enoxil release from composites with pristine fumed silica (*1*), sol-gel silica (*2*) and sol-gel silica with phenyl groups (*3*)

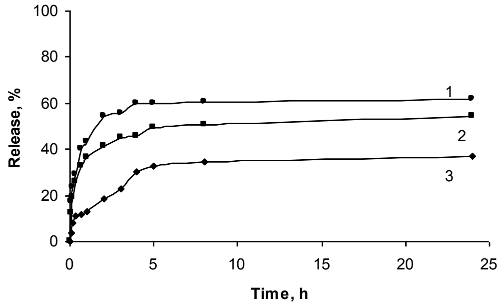

Fig. 2. Enoxil release from polymer films: Gelatin/HEMA-VA (*1*), Gelatin/HEMA (*2*) and Gelatin/Chitosan/HEMA (*3*)

Acknowledgements
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A quantum chemical analysis of dependence of the protolytic properties of polysilicate acids on the composition and spatial structures of their molecules

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High disperse silica is used as a sorbent and carrier of medical preparations in various branches of medicine, biotechnology *etc*. due to its physico-chemical properties, in particular, rather developed surface, chemical inertness, considerable adsorption capacity. The protolytic equilibrium of silica surface is to be examined, because the structure of its hydroxylic layer determines its properties. When silicic acid is polymerized, an increase in the molecular mass of the particles formed, the acidic properties of oligomers are changed.

A quantum chemical analysis of the structure of oligomers of silicic acid containing from 1 to 20 silicon-oxygen tetrahedral has been carried out by density functional theory method with the exchange-correlation functional B3LYP and valence-split basis set 6-31+G(d,p) as well as by semiempirical PM7 method. The effect of aqueous medium was taken into account within the continual solvent model and within the supermolecular approximation.

In order to determine the silica protolytic properties, complexes were designed including the molecules of oligomers mentioned, their silanol groups contacting with four water molecules stationed in the vertices of a trigonal pyramid, in two states – molecular associates and separated ion pairs. The latter is believed to appear due to proton transfer from silanol group to a water molecule so forming a hydronium cation. The spatial structures of these states refer to local minima on the multidimensional potential energy surface.

Starting from the results of calculations of the equilibrium geometry and thermodynamic characteristics of the complexes of silicic acids, one can state that due to a stepwise increase in the number of silicon-oxygen tetrahedral in oligomers a shortening takes place of interatomic bonds as well as changes of atomic net charges reflected in diminishing of the deprotonation constant of silanol groups (pK_a). A correspondence of the calculated constants to related experimental findings suggests a possibility to use the complexes considered for simulation of the protolytic properties of polysilicate acids.

Biological activity and toxicity assessment of polymer/silver composition

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The polymer/silver compositions are a focus of practical interest because of their potential application in biotechnology and medicine. According to the recent publications, these compositions demonstrate unique and enhanced physical, chemical, and biological properties compared to their macroscaled counterparts, thus opening a wide range of their potential applications such as sterilization, disinfection, creation of antibacterial textiles, and drug delivery.

Taking into consideration possibility of wide applicability of polymer/silver compositions as antibacterial agents in fish farming, the present work was focused on assessment of their antibacterial activity against bacterial pathogens of fish.

We evaluated the bactericide action of polymer/silver composition against bacteria *Aeromonas hydrophila* and *Pseudomonas sp.* selected from trout and carp using the agar well diffusion method and the serial broth dilution technique with determination of the minimum bactericidal concentration (MBC).

The polymer/silver composition showed strong inhibitory effects against *A. hydrophyla* (with the zone of inhibition, ZOI, equaled to 22.1±0.2 mm) and significant antibacterial activity against *Pseudomonas sp.* (with ZOI =15.7±0.1 mm). The broth dilution assay gave MBC value of 6 $\mu g \cdot dm^{-3}$ for the polymer/silver composition.

In order to understand, whether polymer/silver composition may pose a threat to non-target species, we estimated the biological risks using environmentally relevant test-organisms such as *Danio rerio*, *Hydra attenuata*, *Daphnia magna*, and *Allium cepa L.* and also the toxicity of the composition to *Danio rerio* embryos, and its gene-toxicity to *Danio rerio* cells.

The result of bioassay indicated that the safe concentration of the polymer/silver composition to all the test-organisms is below 10 $\mu g \cdot dm^{-3}$

Thus, the concentration that showed antibacterial activity did not exhibit the lethal effect and did not cause teratogenicity and chromosomal aberration to all the test-organisms.

These results suggest that the polymer/silver composition could widely be applied as biocide agents in fish farming.

The structure and phase composition of the radiotransparent ceramics

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The most interesting from the point of view of creation of radiotransparent materials is a multicomponent system $SrO–BaO–Al_2O_3–SiO_2$, due to the presence of two crystalline phases in it – Celsian ($BaO·Al_2O_3·SiO_2$) and Slavsonite ($SrO·Al_2O_3·SiO_2$). It is known that Slavsonite and Celsian have high radiophysical and physico-mechanical properties: the permittivity is in the range of 6.2-7, the tangent of the dielectric loss angle is $tg\delta·10^{-4} = 1 – 50$, low TLFE, $\alpha·10^6$ 1/degree = 2.5 – 2.7, peak time melting point is above 1600 °C.

The aim of the work was to justify the choice of the areas of a multicomponent system $SrO–BaO–Al_2O_3–SiO_2$ and to study their structural and phase composition. For this purpose, the effect of the ratio of the crystalline phases of Slavsonite and Celsian (phase ratio $SrAl_2Si_2O_8$: $BaAl_2Si_2O_8$ is: C1 - 1:3; C2 - 1:1 and C3 - 3:1) on the dielectric properties of ceramics were investigated.

It is confirmed that the phase composition of the obtained materials corresponds to the composition of the solid solution, and with the increase of barium oxide in the composition of the masses, the composition of the solution varies from $Ba_{0.5}Sr_{0.5}Al_2Si_2O_8$ to $Ba_{0.75}Sr_{0.25}Al_2Si_2O_8$. A positive effect with the introduction of the second bivalent cation, in particular strontium oxide in the celesium composition, is reflected in the weakening of the growth of the permittivity with increasing temperature. Therefore, it can be considered that the production of thermally stable solid solutions of the Celsian-Slavsonite composition will contribute to an increase in the stability of the dielectric characteristics during the exploitation of the material under conditions of high temperature loads.

The necessity of modification of model masses with the use of intensifiers of sintering and phase formation is established. To ensure the maximum level of sintering, it is recommended to introduce 2 mass. % Li_2O into the composition of masses, which ensures the production at 1450°C of Celsian-Slavsonite ceramics with the following properties: W = 0 %, $\rho_{prop} = 2960÷3025$ kg/m^3; $\varepsilon = 7.3÷8.7$; $tg\delta = 0.0077÷0.0096$; σ_{st}= 110÷180 MPa; σ_{zg}= 15÷35 MPa. Based on the studies carried out in a multicomponent system $SrO–BaO–Al_2O_3–SiO_2$ we have determined the prospective compositions of ceramic materials with a lowered dielectric constant and a tangent of the dielectric loss angle.

Influence of organic solvents on hydration of polylactic acid

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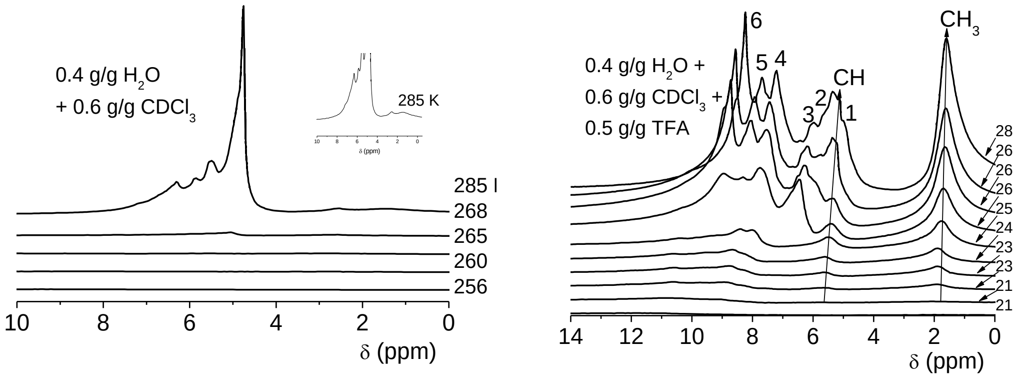
Polylactic acid (PLA), which is a product of polycondensation of *L*-lactide, refers to thermoplastic, biologically inert, biodegradable polymers and is widely used in various branches of industry as a biodegradable material, polymer for 3D printers and antimicrobial films that can be applied directly to food products as well.

To accelerate biodegradation, additional substances that facilitate the penetration of water can be included in the polymer matrix increasing the absorption of ultraviolet light and increasing the adhesion of certain types of microorganisms and fungi.



a

b

Fig. The ^{1}H NMR spectra of water taken at different temperatures in the PLA sample saturated with water for one week (*a*) in the presence of deuterochloroform and in the presence of 0.5 g/g CF_3COOD (*b*)

The state of water in polylactic acid in the presence of deuterochloroform (Fig., *a*) and trifluoroacetic acid (Fig., *b*) was studied by low-temperature ^{1}H NMR spectroscopy. It was shown that the polylactic acid is able to absorb no more than 1 % of water during the first hour and 10 % during the next seven days of saturation with water. Initially water is absorbed in the form of polyassociates and over the time due to the diffusion process is localized near the electron donor sites of the polymer due to formation of hydrogen-bound complexes. When a trifluoroacetic acid is introduced into the system, water-acid clusters with a different acid content are formed in the polymer matrix.

The surface complexes of carboxylic acids and their thermal transformations into important “green” chemicals

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The important route for the conversion of biomass into fuels and chemicals is catalytic pyrolysis, which enables obtaining important intermediates for industrial organic synthesis (ketenes, aldehydes, ketones, alkanes, alkenes, acetylenes *etc*.) from vegetable and algae oils. Fatty acids in the form of triglycerides are promising renewable raw materials for biomass conversion [1-4]. Conversion technologies based on heterogeneous catalysts do not require utilisation of hazardous solvents and are characterised by reduced energy consumption because catalytic reactions take place at significantly lower temperatures. Catalytic pyrolysis can produce biofuels and oleochemicals from the renewable available and inexpensive resources including algae, vegetable oils, agricultural, paper and food-processing industry wastes.

The identification of all types of surface complexes of carboxylic acids on the surface of the potential catalyst is essential for the effective biomass conversion. In present work, the thermal decomposition of carboxylic acids on the surface of nanoscale oxides has been investigated by Temperature-Programmed Desorption Mass Spectrometry (TPD-MS). Fourier transform infrared spectroscopy (FTIR) has been used to investigate the structure of carboxylic acids complexes on the oxide surfaces. Weakly bound forms of carboxylic acids were found to be present on the studied oxide surfaces. These weakly bound surface complexes may play the essential role in the proceeding of thermal transformation of carboxylic acids.

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Synthesis of magnetosensitive composites based on magnetite with carbon-deposited surface

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Porous carbon materials are widely used as sorbents for solution of different tasks in engineering, biotechnology, medicine, environmental protection. Development of this direction got special interest in connection with the synthesis of nanocomposites based on magnetic particles of iron, nickel, cobalt, magnetite in a porous carbon matrix. The aim of this work is the synthesis of magnetosensitive composites based on magnetite with carbon-deposited surface.

For carrying out the carbonization of the magnetite surface the organic substances – oleic acid (sample 1 – 0.5 g Fe_3O_4, 1 ml of oleic acid); Poligel CS (Carbomer 934) (sample 2 –0.5 g Fe_3O_4, 1 ml of 3% Poligel CS solution) were used. Nanodisperse magnetite was impregnated by solution of oleic acid and 3% Poligel CS solution at room temperature. After drying at temperature of 115°C, the matrix with adsorbed organic matter was obtained, annealed at 400°C for 2 h in a stream of argon.

Sorption capacity was evaluated by adsorption of methylene blue. For the experiment a portion of the sorbent 30 mg was taken, which was filled with 5 ml of an aqueous solution of methylene blue in concentration range: 0.003 – 0.02 mg/ml. Optical density of the solutions before and after adsorption were recorded on FEC 2, at a wavelength of 590 nm and cuvette thickness l = 0,5 cm. Sorbent and dye were kept for an hour, then the sorbent was separated by decantation on the permanent magnet. The amount of adsorbed substance on the surface of the composites was determined by measuring the concentration of the contact solutions before and after adsorption according to the calibration schedule. According to studies of the built adsorption isotherm, the extraction degree (R%) and an indicator of adsorption capacity A (mg/g) were calculated.

R indicator for sample 1 is 22% and for sample 2 - 54%.

Conclusion: there is a prospect of the synthesized nanocomposites to create adsorbents of biomedical, technical and environmental purposes.

Hygroscopicity of the composites with various Enoxil-to-silica ratios

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Recently, much attention is focused on a study of bioactive compounds of plant origin with antibacterial and antioxidant properties. Such a kind of the compounds in a relatively novel preparation (Enoxil) was obtained by the oxidation of tannins extracted from grape seeds and it was found to possess high antibacterial and antioxidant activity. The Enoxil is a mixture of monomeric derivatives of catehine and epicatehine in the free form and esterified with gallic acid as well as with peroxidic compounds. Due to high content of hydrophilic groups, Enoxil is characterized by enhanced hygroscopicity, which, in turn, requires special conditions for its storage or inclusion in formulation preventing excess water uptake.

It is known that highly dispersed silica may be used in the drug composition as a carrier of biologically active substance, which also decreases the hygroscopicity of the latter. In the previous study we did reveal a decrease in Enoxil hygroscopicity when this preparation was dispersed at silica surface. The aim of this work was to prepare the Enoxil-silica composites with various Enoxil-to-silica ratios and to examine the effect of silica content on water absorption by these composites.

Fumed silica with S_{sp} of 300 m^2g (A-300, Kalush, Ukraine) was mechanically mixed with Enoxil powder (produced at the Institute of Chemistry, Academy of Sciences of Moldova). The Enoxil-to-silica ratio was varied within 0.1÷1.0 range. The capability of Enoxil, silica and Enoxil-silica composites to absorb water from the gas phase was determined gravimetrically by the sample mass change before and after holding in an exsiccator. The data on water absorption by each composite was compared to the theoretically calculated amount of water which would be absorbed by the composite in the case when individual components do not affect the water absorption by each other.

For all the composites studied, the water absorption was found to be less than that for the Enoxil powder. The largest decrease in hygroscopicity was observed for the composites with Enoxil-to-silica ratio of 0.1÷0.2, corresponding to the approximate Enoxil monolayer formed at silica surface. Thus, the approach to prepare Enoxil-silica composites was found to be suitable for decreasing the Enoxil hygroscopicity and for improvement its storage stability.

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Features of inorganic nanoparticles modeling. Nano-QSAR for cytotoxicity of metal oxides

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Nano-QSAR modeling is a modern and effective tool for investigating the structure-properties relationships for various nanosystems. Features of modeling nanoparticles require taking into account not only the structure of molecules forming a nanoparticle, but also the characteristics of the nanoparticle itself. In addition, well-known systems of 2D descriptors for organic molecules are not applicable to inorganic compounds. The reason for this is the incorrectness of the description by the structural formulas of many inorganic substances in the crystalline state. Thus, it becomes necessary to develop specific approaches for describing inorganic nanoparticles for subsequent QSAR analysis.

In this work, the system of 1D descriptors for the representation of inorganic substances in QSAR models is developed. These descriptors based on the fundamental characteristics of atoms (nuclear charge, oxidation level, electronegativity, ionic radius, ionic refraction *etc*.) and taking into account the number of different combinations of atoms (doublets –A_2, AB, …, triplets – A_3, A_2B, ABC, … *etc*.) in gross-formulae for an inorganic substance. For the characterization of nanoparticles themselves, the "liquid drop" method developed earlier was used [1]. From this method we estimate such parameters: assumed number of molecules in the nanoclaster, volume of nanoclaster, surface area of nanoclaster, number of surface molecules, surface molecules ratio.

The effectiveness of the proposed approach is demonstrated by the example of a study of cytotoxicity of 17 metal oxide nanoparticles (ZnO, CuO, V_2O_3, Y_2O_3, Bi_2O_3, In_2O_3, Sb_2O_3, Al_2O_3, Fe_2O_3, SiO_2, ZrO_2, SnO_2, TiO_2, CoO, NiO, Cr_2O_3, La_2O_3) against *E. coli* and *HaCaT* cells [2]. The obtained QSAR models are quite adequate and have predictive power. The main structural factors determining the cytotoxicity of nanooxides were revealed.

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Features of the interaction between InAs, InSb, GaAs and GaSb and $(NH_4)_2Cr_2O_7{-}HBr{-}C_4H_6O_6$ mixtures

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The investigation results of the mechanism and kinetics of the interaction between InAs, InSb, GaAs, GaSb and $(NH_4)_2Cr_2O_7{-}HBr{-}C_4H_6O_6$ solutions have been presented and the quality of the obtained surface has been examined. The InAs (001), GaAs (111), InSb (112), GaSb (112) substrates were cut from the single-crystalline ingots using string cutting with diamond coating.

In order to decrease the damaged layer, the crystals were previously mechanically grinded and chemical-mechanically polished (CPM). The interaction between the semiconductors and the $(NH_4)_2Cr_2O_7{-}HBr{-}C_4H_6O_6$ etchants was studied using the chemical-dynamic polishing (CDP). The semiconductors dissolution rates changed as follows: the 0.05 μm/min minimum value was achieved at the maximum $C_4H_6O_6$ concentration; in the $(NH_4)_2Cr_2O_7$ enriched solutions the maximum of the etching rate was achieved (7.5 and 5.6 μm/min – for InAs and GaAs; 7.9 and 8.4 μm/min – for InSb and GaSb). The analysis of the etching rate changes shows the similarity between the dissolution mechanisms of InAs and GaAs, as well as InSb and GaSb. The obtained dependencies of the CDP rates on the solution temperature and stirring speed suggest that the substrates dissolution mechanism is diffusion-limited.

The surface microstructure after treatment was studied using HOMMEL-ETAMIC W5 profilometer and AFM. The InAs surface had the longitudinal stripes and the microcracks after string cutting (R_a=1200 nm). The rough surface with R_a=30 nm was obtained after ASM 1/0 grinding. After CMP and CDP the surface was mirror-like with R_a = 0.2 and 3.3 nm, accordingly (Fig.).

a ***b***

Fig. The surface ASM-images of InAs (*a*) and InSb (*b*) after CDP in the $(NH_4)_2Cr_2O_7{-}HBr{-}C_4H_6O_6$ solution

Analysis of the ASM results suggests that the $(NH_4)_2Cr_2O_7{-}HBr{-}C_4H_6O_6$ etchants promote more quality polishing surface of arsenides in comparison with antimonides.

$CuAlO_2$ films formation using the reactive ion beam sputtering method

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The synthesis of semiconductors of *p*- and *n*-type conductivity with a band gap greater than 3.1 eV is an urgent task of creating devices of transparent electronics (TE) [1]. Zinc oxide is the wide direct band gap (E_g =3.3 eV) *n*-type semiconductor material which can be used in TE as passive (conductive contacts, resistors) and as active (material for *p-n* junction) element. However, the achievement of *p*-type conductivity in ZnO is a main challenge on the way of creating a ZnO-based TE. The use of *p*-type $CuAlO_2$ (E_g = 3.5 eV) is a possible solution to the problem of creating a *pn*-heterojunction with ZnO. The actual problem of the growth of $CuAlO_2$ films is the formation of thermodynamically stable undesirable phases like Cu_2O, CuO, Al_2O_3 and $CuAl_2O_4$.

Al-Cu-O films were deposited on Si (111) and glass substrates by reactive ion beam sputtering method of floatable Al-Cu target with atomic ratio of 1:1. The substrate temperatures were changed in the range 80-380 °C at fixed other technological parameters. As-grown samples were annealed at 900 °C under atmospheric conditions during 3 h. After that, one series of samples was cooled at slow rate (during 3 h) and the second one was done at fast rate (during 15 min.

The properties of as-grown and annealed films were studied by using X-ray diffraction, energy dispersive X-ray spectroscopy, atomic force microscopy, Fourier transform infrared spectrometry and optical transmission measurements. In our report the influence of substrate temperature and annealing treatments on the structure, optical properties, elemental composition, and surface morphology of samples were investigated and discussed in detail.

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Supramolecular interactions of natural flavonoids with anticeptic cationic surfactant ethonium in solutions and on the silica surface

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Supramolecular interactions of structurally related flavonoids, quercetin (3,5,7,3',4'-pentahydroxyflavone) and rutin (5,7,3',4'-tetrahydroxyflavone-3-rutinoside) with anticeptic cationic surfactant ethonium (aethonium, etonium, 1,2-ethylene-*bis*-(N-dimethylcarbdecyloxymethyl) ammonium dichloride were studied spectrophotometrically. By its structure ethonium belongs to dimeric surfactants, containing two head groups and two aliphatic chains – “tails”, linked by a rigid or flexible space. This surfactant was considered to be a promising solubilizer for flavonoids studied. Quercetin and rutin have potent antioxidant and metal ion chelating capacity, possess various biological and biochemical effects including anti-inflammatory, antisclerotic, antineoplastic, spasmolytic, diuretic and cardio-protective activities, but their application is limited because of low solubility.

Physico-chemical studies have shown that addition of ethonium to flavonoid aqueous solutions causes alteration of their spectral and acid-base properties, increases solubility and adsorption on silica surface. The bathochromic shift of quercetin and rutin spectra in pre-micellar ethonium solutions testified an increase in their polarity. Indeed, the calculated values of their apparent dissociation constants in ethonium solutions were lower than in water. In micellar solutions after reaching critical micelle concentration the flavonoid spectral characteristics and protolytic properties remain unchanged, whereas the solubility of quercetin and rutin raises 250 and 5 times, respectively.

The formation of supramolecular complexes also causes the essential increase of quercetin and rutin adsorption on silica surface at pH>5 both in pre-micellar and micellar ethonium solutions in similar ways. This allows to assume that the structure of surface complexes formed by pre-micellar associates and micelles has no principal differences. The shape of the obtained pH-dependences of quercetin and rutin adsorption suggests that flavonoids as a part of ethonium supramolecular complexes area dsorbed on silica mainly through the ionic interactions between the positively charged nitrogen atoms and dissociated silanol groups. The results of physico-chemical study may be a base for the development a composition of new medicinal remedies.

Synthesis and characterization of N-doped TiO_2 nanospheres

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Titanium compounds (oxides, dioxides *etc.*) are commonly used in a wide range of applications including catalysis, sorption and electrochemistry. Such parameters as surface area values, porosity and the presence of functional groups are of great significance in these cases. Procedures of doping TiO_2 by nitrogen are well known and allow for obtaining samples with tailored phisico-chemical characteristics. Nitrogen, nitrogen-containing salts and surfactants are the most appropriate reagents in the practice of doping.

The aim of this work was the search for correlations between the parameters of synthesis of N-doped TiO_2 samples and their phisico-chemical characteristics.

It has been shown that the key conditions of synthesis are TiO_2:urea ratio and pH of the solution. For comparison, Ti^{4+}:urea ratios such as 100:2.5 (sample I), 100:5.0 (sample II) and 100:10.0 (sample III) have been used. The ammonia solution has been employed as a precipitant. Due to the formation of a buffer mixture, the precipitation of sample III fails. It should be mentioned that the sample II becomes yellow upon heat treatment at 400 °C, proving the effect of doping by nitrogen.

Phisico-chemical characteristics of the samples obtained have been investigated by SEM (Jeol 6700F, Japan), XRD (CuK_α radiation) and porosity techniques. It has been shown that the specific surface area for the samples lies in the range of 396-410 $m^2 \cdot g^{-1}$, whereas upon heat treatment at 400 °C it decreases to 113-124 $m^2 \cdot g^{-1}$. Prevailing pore size is 1.7-1.8 and 2.2-2.4 nm before and after manipulations. In accordance with XRD data, the anatase structure has been observed for sample II with an average crystal size of 7.6 nm. The particles of the doped unheated sample are nanosized and spherical in shape (Fig., *a*, *b*). Treatment at 400 °C results in increasing particle size (Fig., *b*).

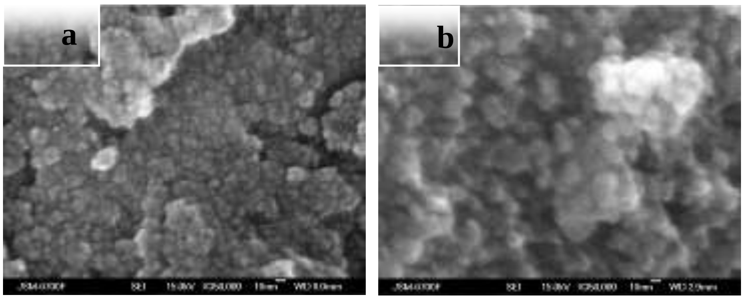

Fig. SEM micrographs of samples before (*a*) and after heat treatment (*b*)

Synthesis of graphene nanoplatelets/(Ni-Co) composites and their properties

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Graphene structures are rising in practical use and research, due to the complex of unique properties, high performance, low cost, manufacturability. Technologies of obtaining high-quality materials and composites that consist of graphene nanoplatelets (GNP) is an important direction of development modern materials.

The aim is to develop a method of synthesis system GNP/(Ni-Co) and to study the physical and chemical properties of the composites.

GNP is obtained by electrochemical deposition in a low electrolyte (KOH) concentration by passing a current of 6.0 to 60 mA/cm^2. Composites GNP/(Ni-Co) were obtained at a temperature of 80^{o}C by co-precipitation of an aqueous solution of crystalline carbonate in hydrazine hydrate of nickel and cobalt and suspensions GNP.

The results of X-ray diffraction analysis conducted on the diffractometer DRON-4.7, indicate the presence of GNP phases, cubic system nickel, cobalt hexagonal crystal lattice, the absence of reflexes incoming carbonates. By the method of thermogravimetry (Derivatograph Q-1500 D) it was found that the oxidation of metals in composites begins at the 295^{o}C temperature and oxidation GNP at the 600^{o}C. There were metal particles sized ~40-50 nm found on the GNP surface by using transmission electron microscopy (JEOL JEM 1230).

Gas sensory properties of composites in acetone and ammonia are unstable. There is intense oxidation of the samples with irreversible loss of properties. Composites are susceptible to ethanol vapor, the relative resistance in the presence of alcohol increases by about 25%. Specifications are regenerative over numerous cycles.

Electrical properties of the composites were researched at low frequencies by using a spectrometer Solartron SI 1260. Conductivity at a room temperature reaches up to the values of 0.44 Ohm$^{-1}\cdot$cm^{-1} with the dispersed component density 2 g/cm^3. The samples have expressed magnetic properties and a magnetic permeability at a frequency of 100 kHz about 10.

The resulting nanocomposites can be promising devices for use in energy conversion, catalysis, gas sensor, screening and magnetic devices.

Intermolecular interactions of like-charged oligomeric electrolytes and surfactants in aqueous media

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Implementation of autoclave technology for the production of non-ferrous metals became possible due to the use of surfactants capable of eliminating the concomitant film formation of the sulfur element on the surface of ore particles. As a surfactant, technical lignosulfonates (LS) are used, the effectiveness of which is inadequate and worsens over time. Therefore, it is of industrial importance to develop new surface active compositions.

In the present work, it is proposed to use the same-charged oligomeric electrolytes of LS in a mixture with sodium dodecyl sulfate (DSNa). LS-NMF fractions (M_w = 9250 amu), VMF (M_w = 46300 amu), and DSNa ($C_{12}H_{25}SO_4Na$) of the grade chemically pure were used. In the solutions the concentrations of C_{LS} 0 ÷ 0.64 g/dm^3 and CDSNa 0 ÷ 0.64 g/dm^3 were varied. The optical density, the electrical conductivity, surface tension in the temperature range 16 - 75 °C were determined.

It was established that the mixtures of LS-DSNa-H_2O are transparent, the formation of new micro- or macrophases was not observed.

It was shown that for all the binary mixtures studied, the specific electric conductivity increases with increasing concentration of both LS and DSNa. The values of the equivalent electrical conductivity of binary solutions are greater than the additively calculated value, which indicates the synergy of the mutual influence of the components on the electrical conductivity of the system.

It was found that when the concentration of LS is increased at a constant concentration of DSNa, the surface tension of the solutions decreases, and the decrease in σ-*r* is more important the higher is the solution temperature.

Thus, a change in the physico-chemical parameters of the system indicates an effective interaction in LS mixtures with the anionic surfactant DSNa.

Regularities of hydrogen evolution from water at modified tungsten carbide based cathodes

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The high electrocatalytic activity of tungsten monocarbide (WC) in cathodic hydrogen evolution from water is well known. In the present work, some WC based electrodes, modified with silver, copper or titanium, have been made at different conditions and investigated as cathodes for hydrogen evolution from acid and alkaline solutions.

Fine (6 µm) WC powder, mixed with silver (5, 10 and 20 wt. %) or copper (5, 10 and 20 wt. %) or titanium (10 wt. %) powder, was used for the preparation of the electrodes. Mixtures of metallic powders with an aqueous solution of polyvinyl alcohol were applied on a nickel mesh, dried and fritted under argon. The fritting temperatures were 900 °C (WC, WC + Ag, WC + Cu), 1100 °C (WC + Ti) and 1350 °C (WC, WC + Ag). The regularities of cathodic hydrogen evolution at the prepared composite electrodes were studied in 1 M H_2SO_4 and 1 M KOH solutions by recording slow ($2\ mV{\cdot}s^{-1}$) polarization curves.

It has been found that all investigated electrodes were more active in the electrolysis of acid solution than of alkaline one, regardless of the temperature of electrode fritting and modifying dope. The lowest overpotential of hydrogen evolution was recorded at a WC electrode modified with 5 wt. % Ag in an acid solution (217 mV at a current density $100\ mA{\cdot}cm^{-2}$ and temperature 25 °C). Titanium doping in WC electrodes also led to some decrease in hydrogen overpotential while at WC + Cu electrode hydrogen was evolved with overpotential higher than at unmodified WC electrode.

The lowest activation energy ($13.3\ kJ{\cdot}mol^{-1}$) was established when hydrogen was evolved from an acid solution at a WC electrode modified with 5 wt.% Ag. Tafel coefficient *b* had approximately the same value when hydrogen was evolved at all investigated electrodes, which indicates that the mechanism of hydrogen evolution at these electrodes was identical.

Increasing Ag content in WC + Ag electrodes from 5 to 20 wt. % insignificantly influenced electrode activity, therefore the doping of WC with more than 5 wt. % Ag is inexpedient. Lowering the fritting temperature from 1350 to 900 °C did not impair the kinetic parameters of hydrogen evolution at WC and WC + Ag electrodes. At the same time, electrodes fritted at 900 °C were sufficiently strong and unbreakable.

Simple models and equations of adsorption kinetics in practical application

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Adsorbents are widely used in industrial processes as well in environment protection applications – here we focus on applications in aqueous solutions. The basic requirements for an appropriate adsorbent are defined mainly by parameters describing its structural and surface properties that may be determined by using gas (typically nitrogen) adsorption data analysis. Equally or sometimes even more important are its properties derived from equilibrium adsorption isotherms of particular substances of interest in specific process conditions (solvent, i.e. water, effect of pH on adsorbent and adsorbate, presence of other chemical species).

The specific adsorption system properties that may be derived from equilibrium data are often insufficient to guarantee efficiency of actual industrial operations and water/wastewater processing. In such applications appropriate mathematical description and understanding of adsorption rates is a crucial factor. For many systems advanced modelling is too costly and impractical, hence simple models as well as semi-empirical and empirical equations are generally employed to analyse adsorption kinetic data. In fact for simple models, simplification of system properties is required, which leads to obtaining model parameters that are in fact composite constants without simple possibility to extract corresponding component parameters. It essentially makes such models equivalent to semi-empirical equations. For example parameters of IKL equation (Langmuir kinetics) should be in agreement with those of equilibrium isotherm (Langmuir isotherm) – if not, then mathematically equivalent 1,2-mixed order equation (MOE) can be used to describe the same data (first and second order equations are boundary cases of IKL and MOE) [1-3]. Similarly, intraparticle diffusion models show also similar deficiencies in practical applications [3-5].

Acknowledgements

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Study of dyes adsorption on carbon materials in the multicomponent system

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One of the most important problems of the modern world is water pollution. Intense industrial development and continuing urbanization have caused excessive toxic emissions including dyes and pigments. These substances are widely used in the textile industry, paper, rubber, plastics, leather, cosmetic, pharmaceutical and food. Dyes are relatively well soluble in water, resistant to biodegradation, while usually toxic and carcinogenic [1-3]. Therefore, they should be carefully removed from the water and sewage.

Adsorption methods are commonly used in the process of purifying water and wastewater from toxic substances. The use of active carbon as an adsorbent allows for efficient removal of impurities, especially organic ones [4-6]. The efficiency of the adsorption process depends on many factors, where the presence of competing substances is a prominent one [7].

The main aim of this study was examination of adsorption of dyes on carbon materials in the multicomponent system by applying UV-Vis spectrophotometry. Adsorption isotherms and concentration profiles have been experimentally determined and analyzed by using several simple equations.

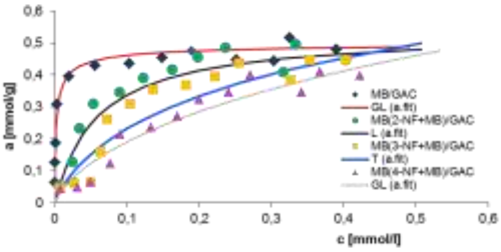

Fig. Comparison of adsorption kinetics of MB on GAC in single- and multi-component systems

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Synthesis and electrical properties of CuI/Fe_3O_4–polychlorotrifluoroethylene nanocomposites

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The development of science and technology stimulates the creation of new functional polymer composite materials (PCM) with high operational parameters under the conditions of various physical fields. To such materials belong, in particular, PCM on the basis of active components with electron-ionic conductivity and magnetite.

The samples necessary for the studies were prepared by a chemical method for modifying magnetite with copper iodide during the course of release of CuI from an aqueous solution of $CuSO_4$ and KI, $Na_2S_2O_3$ in the presence of Fe_3O_4 to obtain modified magnetite (CuI/Fe_3O_4). Original Fe_3O_4 and composites CuI/Fe_3O_4 were investigated by X-ray analysis (XRD), transmission electron microscopy (TEM). The real (σ') and imaginary (σ'') components of the complex electrical conductivity ($\sigma^*=\sigma'+i\sigma''$) at low frequencies (0.1, 1 and 10 kHz) were measured using the immittance meter E7-14 by two-contacts method in the temperature range from 298 to 425 K. The real (ε') and imaginary (ε'') components of the complex permittivity in microwave range were measured using the interferometer at a frequency of 9 GHz. The samples of system CuI/Fe_3O_4–polychlorotrifluoroethylene (PCTFE) was compacted at the temperature equal to the melting point of the polymer (523 K) at a pressure of 2 MPa.

Our identification of the observed diffraction XRD maxima provides evidence for the fact that in the samples CuI/Fe_3O_4 there is a copper iodide cubic and hexagonal modification. Besides, it is seen that the major reflection intensity increases in proportion to the content of CuI in the samples. The calculation results indicate that with increasing CuI content bulk in disperse systems from 0.27 to 0.58 volume fraction the crystallite size increases from 8 to 12 nm. Surface modification of magnetite, CuI leads to a significant increase in the values of ε', ε'' and σ of both the low and high frequencies. Observed a significant increase in the values of ε', ε'' in the concentration dependence of CuI/Fe_3O_4 for the content bulk of copper iodide > 0.27. It should be noted that the dependence of ε' and ε'' on the concentration of CuI of system CuI/Fe_3O_4 have a maximum in the concentration of ~ 0.4. Introduction of CuI/Fe_3O_4 in the polymer leads to increased values of complex permittivity in the microwave range. Maximum values of complex permittivity and conductivity for a system CuI/Fe_3O_4–PCTFE were determined at a concentration CuI ~ 0.27.

Gold clusters generated with laser desorption/ionization

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The surface chemistry of gold nanoparticles (NPs) can be modified with different agents to perform wide array of functions. For application of Au NPs in medicine their toxicity must be reduced. This effect can be achieved when amino acid tryptophan (Trp) is used for the synthesis of NPs as reducing and stabilizing agent.

Three different combinations of reagents were used to produce gold NPs: 1) $NaBH_4$ as reducing agent and surfactant SDS as stabilizer; 2) $NaBH_4$ as reducing agent and Trp as stabilizer; 3) Trp for both purposes. All obtained gold colloids had inherent color and localized surface plasmon resonance band in absorption spectra.

We showed similarities and differences in fragmentation of Au NPs obtained by different ways by laser desorption/ionization mass spectroscopy. Au NPs mostly decompose during ionization process. For all systems in mass spectra for positive and negative ions, the series of intense single monoisotopic peaks with a pitch of 197 Da that refers to the average mass of Au were observed (Fig.). The intensity alternation of clusters having even and odd number of atoms is discussed.

Amino acid tryptophan as bifunctional agent satisfies the synthetic approach to obtain nanosized gold, as well as reduces its toxicity.

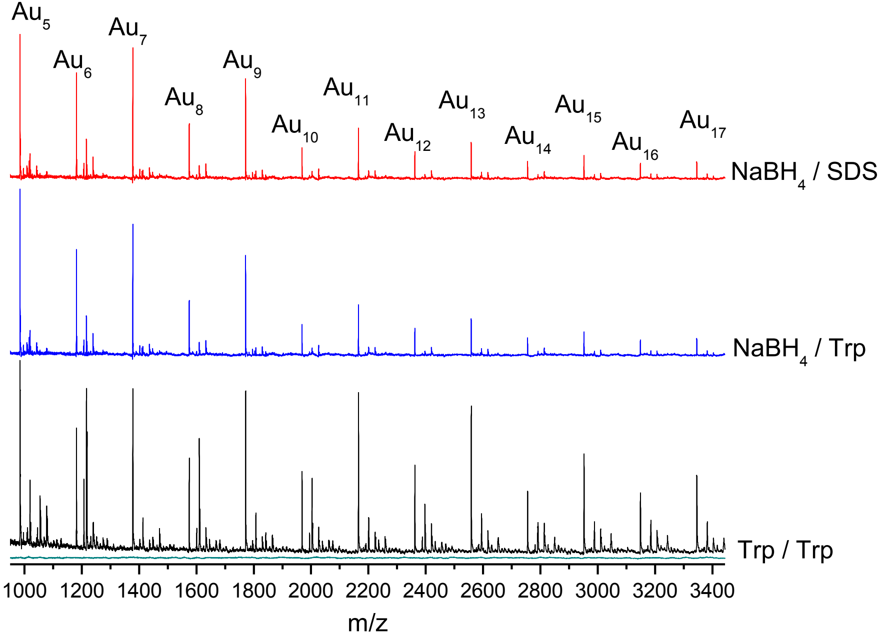

Fig. Representative fragment of mass spectra of gold colloids under consideration in mass range 1000 to 3400 Da for negative ions (reflectron)

Double-layer silicene as a molecular container for anti-aromatic systems

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Silicene is a newly discovered material which is one atomic layer thin. It is a two-dimensional (2D) nanomaterial that is classified as a nanosheet which has large lateral dimensions up to micrometres, but thickness of several nanometres or less. The unique properties and morphology of such materials make them ideal for a variety of applications, including electronic devices, batteries and sensors. 2D nanosheet of silicene can be considered as analogue of graphene. The specific surface area of nanomaterials can play one of the key roles in their application [1-5].

Our main object of interest – a double silicene layer – was modelled with 32 silicon atoms in each plane. The distance between the planes was chosen to be 0.3855 nm (we selected the AB… order of silicon atoms between the planes). Double-layer silicene intercalation is produced via introduction of the intercalate molecules into the inter-layer space. As stated above, our goal was to study the system of two silicene planes, with cyclobutadiene molecules intercalated between them. Of particular interest are the positions of the cyclobutadiene relatively each other and the silicon atoms, mutual positioning of the silicene planes in the presence of the cyclobutadiene intercalates (with or without keeping the AB… order of silicone atoms between the planes), as well as the stability of the system under thermal treatment.

The computation was made by MM+, PM3 and Monte-Carlo methods. The association constant is as follows: $K_{ass} = 380\ \mathrm{l{\cdot}mol^{-1}}$, with computation accuracy $k_{korr} \geq 0.977$.

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DFT study on reactivity of graphite carbon atoms in basal-plane positions

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Oxidation of natural and synthetic graphite materials is a long-term research topic due to increasing safety requirements in nuclear power sector where they are used. Early study by J.M. Thomas [1] demonstrated the anisotropy of the natural graphite surface to oxidation. It appeared that the rate of graphite surface oxidation with O_2 at 1073 K was 26 times lower in the perpendicular direction to the basal plane than that in the parallel one. Hence, the basal carbon atoms are much less reactive than those in the edge sites.

The aim of this work is a quantum chemical simulation of the reactivity of graphite carbon atoms in basal-plane positions with respect to molecular oxygen.

We applied density functional theory (DFT) to analyse the formation of oxygen-containing functional groups resulting from hypothetical reaction of oxygen molecule with graphite carbon atoms in basal-plane position. All calculations have been carried out using the B3LYP exchange-correlation functional and valence-split basis set expanded with polarization functions (3-21G**). For all considered cases the dependence of Gibbs free energy on the temperature was calculated. One particular example of the considered oxygen-containing graphite surface groups formed as a result of hypothetical graphite reaction with oxygen molecule $C_{80}H_{22} + O_2 \rightarrow C_{80}H_{22}O_2$ is illustrated in Fig.

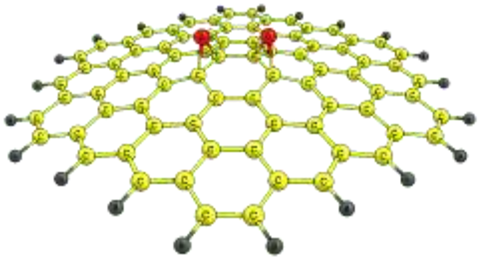

Fig. Example of oxygen-containing graphite surface groups ($C_{80}H_{22}O_2$ cluster)

It appeared that in the temperature interval from 600 to 1500 K the values of the Gibbs free energy for all the reactions were positive and varied from 291.3 to 518.7 kJ/mol. This means that all considered hypothetical reactions of the formation of oxygen-containing functional groups resulting from of oxygen molecule interaction with graphite atoms in basal-plane positions were energetically unfavourable.

The results of undertaken DFT simulation show that interaction of molecular oxygen with graphite cannot lead to the formation of surface oxygen-containing groups on basal plane and so should not be considered as the first stage of deep graphite oxidation.

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Comparative characteristic of sorption properties of mesoporous silica with thiourea ligand towards heavy metals

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Surface functionalization of mesoporous materials widens the range of their application in biotechnology, medicine, catalysis, and in the sorption of heavy metals (mercury, silver, cadmium, lead). There are different ways of functional groups introduction. For example, original SBA-15 can be modified with trialkoxysilanes or using two-component systems during its single-stage synthesis.

The surface layer of such adsorptive materials can bind metal ions in stable complexes. In our previous work, we developed a technique for the synthesis of mesoporous SBA-15 type silica with –NH–C(=S)–NH– groups [1]. Thus, for the sample TEOS:trifunctional silane = 10:0.5, the sorption equilibrium is reached within 30 min. Kinetic characteristics of sample with TEOS:trifunctional silane = 10:2 are much worse, but as expected, with an increase in the concentration of thiourea groups in the mesoporous samples, their static sorption capacity (SSC) increases. Maximal SSC to silver(I) – 192 mg/g and mercury(II) ions – 403 mg/g, cadmium(II) ions – 390 mg/g. Interestingly, that thione form of thiourea groups prevails on the pore surface of mesoporous samples at all TEOS: trifunctional silane ratios. However, during the sorption of mercury(II) and silver(I) ions, thione form transits into thiol, and the formation of 1:1 sulfide complexes is observed. This is accompanied by the decrease in the pH of the sorption solution. In addition, all the IR spectra contain absorption bands inherent to the nitrate ion, which compensates the charge of the complex formed in the surface layer. Therefore, it could be argued, that there is an ion exchange (thiol protons are replaced by metal cations), however thiol sulfur is binding metal ions via coordination bonds.

The pH dependence of the adsorption degree was studied, which exhibited maximum at pH 4.0 and the sorption equilibrium is reached within 3 h. In addition, the kinetic parameters of the adsorption process were evaluated, and the adsorption of cadmium(II) ions in the static conditions was analysed.

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Investigation of the degree of binding and controlled release of doxorubicin from the surface of UDD and OLC

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The aim of the study was to investigate the degree of binding and the possibility of controlled release of doxorubicin (DOX) from the surface of carbon nanomaterials (CNMs). Another goal was to analyze cytotoxic effect of the obtaining materials on tumor cells *in vitro*.

Cellular adenocarcinoma cell line (MCF-7) and hepatocellular carcinoma (HT29) were used as cellular models. The cells were incubated under standard conditions, in 5% CO_2, 95% humidity, in RPMI 1640 medium (Sigma, USA). As carbon nanomaterials, ultra-dispersed diamonds (UDDs) and onion-like carbon (OLCs) were used. UDD and OLC were obtained by detonation synthesis, purified and oxidized. For the oxidation of CNM, the method of incubation in 70% HNO_3 at 100 °C for 4 h was used. Immobilization of DOX on the surface of oxidized UDD and OLC was carried out by sequential treatment with solutions of bifunctional water-soluble crosslinking reagent - carbodiimide (N-(3-dimethylaminopropyl)-N-ethylcarbodiimide hydrochloride, Sigma) and Doxorubicin-lactose monohydrate (Teva Pharm., USA). A proteolytic enzyme trypsin was used for the dose-dependent release of DOX in a runoff concentration of 0.25 mg per 100 ml (0.25 g/v). In result, for the UDD-DOX complex, at concentrations 0.2-0.3 μg/ml, the concentration of free DOX was 3.22 μg/ml at 0.6-3.75 μg/ml, respectively, 6.5-6.8 μg/ml, and at 5.0 μg/ml of trypsin the concentration of free DOX rose to 11.31 μg/ml. For the OLC-DOX complex at concentrations of trypsin 0.2-0.6 μg/ml, the concentration of free DOX was 6.0-6.0 μg/ml, at 1.3-2.5 μg/ml, 7.6-7 7 μg/ml DOX, and at 5.0 μg/ml trypsin, the concentration of free DOX reached 12,18 μg/ml. Survival of adenocarcinoma cells (MCF-7) after incubation with UDD-DOX decreased from 52 to 28% (concentration of UDD from 8.4 to 670 μg/ml, DOX from 2.5 to 20 μg/ml) for 24 h. Incubation with OLC-DOX at the same conditions leaded to decreasing MCF-7cell viability from 72 to 30%. The sensitivity of the cells of hepatocellular carcinoma (HT29) to DOX was higher than that of MCF-7 cells. So, we can conclude that, carbon based nanoparticles (UDD and OLC) are perspective carriers for controlled drug delivery and release.

Effect of mechanoactivation conditions on bulk density of fumed silica

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A number of parameters of fumed silica change during mechanical activation in a ball-mill in the air atmosphere. One of them is changes in the bulk density of nanosilica (d_{bulk}). We carried out gas-phase mechanoactivation of nanosilica in the presence of water and ethanol vapor to intensify the process of modification. To realize this process, water or ethanol was added to the volume of the ball-mill in the amount of 500 mg per 1 g of nanosilica. In this case, nanosilica remains in the powder state similar to that of the initial material. The presence of water or ethanol in the ball-mill influences the process (Fig.).

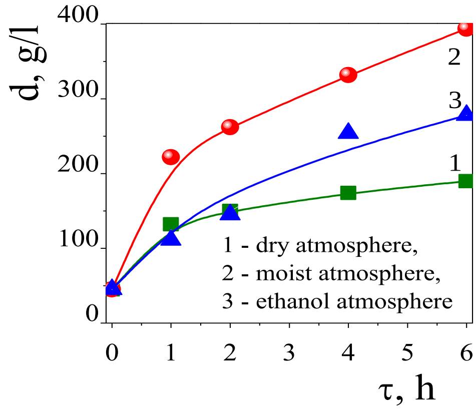

Fig. Dependence of the bulk density of nanosilica on the atmosphere and time of mechanoactivation

Obviously, water or ethanol exists partly in vapor form and as an adsorbate on a surface of nanosilica. By comparing the amounts of water and ethanol added into the ball-mill and desorbed ones from the samples after mechanoactivation, a ratio was estimated. For water or ethanol, 75 or 45 wt.% is on the silica surface and 25 or 55 wt.% in the gas phase, respectively. Perhaps, this is one of the reasons of a greater efficiency of water as an agent contributing the process of geometric modification of nanosilica.

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Adsorption removal of anthocyanins from red cabbage extracts by bentonite: statistical analysis of main and interaction effects

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During the last years, numerous studies about biological activities of anthocyanins have been published. Red cabbage has high anthocyanin content. In comparison to other common plants (berries, fruits, and vegetables) rich in anthocyanins this vegetable can be to become the very cheap source of anthocyanins, because it yields quickly and its cultivation, harvest, and storage are not difficult.

Adsorption is an efficient method that achieves the high yield of anthocyanins from plant extracts while preserving the biological activity and colour of anthocyanin molecules.

The aim of current study is to establish how contact time (τ), temperature (t), initial anthocyanin concentration (C), adsorbent mass (m) ultimately affected on anthocyanin removal efficiency from red cabbage extracts by bentonite. A factorial design 2^4 was used to analyze main and interaction effects of the factors on anthocyanin removal.

Anthocyanin extract of red cabbage leaves was prepared by maceration using 0.1 M HCl. The adsorbent was bentonite from Dashukovsky deposit (Ukraine).

Studies have shown that the factorial design analysis is an important tool and can be used in order to obtain a mathematical model to predict the adsorption removal of anthocyanins from red cabbage extracts. It was determined that all investigated factors and their interactions affect the efficiency of adsorption removal of anthocyanins from red cabbage extract. In this study, we obtained the mathematical model that defines the connection between the removal efficiency of anthocyanins from red cabbage extracts and four control factors. The model can be used for prediction of the adsorption removal of anthocyanins considering optimal conditions of adsorption.

It was concluded the time and adsorbent mass have positive influence whereas initial anthocyanin concentration and temperature have the negative influence on the adsorption removal of red cabbage anthocyanins. Interactions effects are essential for 2-way interactions τt and 3-way interactions τCm and tCm that have the negative influence on the anthocyanin adsorption from red cabbage extract on bentonite.

Structure and optical properties of Nd_2O_3–, $Nd_{9.33}Si_6O_{26}$–fumed silica composites

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At present, neodymium-containing composites are used in various fields of technology as materials for lasers, solid state fuel cell, ceramics and others because of their optical, electrical, chemical and mechanical properties. Composites obtained via solid-phase reactions of fumed silica and neodymium oxides at temperatures near 1000° C are powder materials. Their properties are largely determined by the properties of the neodymium compounds. Thus composites $Nd_{9.33}Si_6O_{26}/SiO_2$ have ionic conductivity at a certain content of components. According to the literature they presumably can be candidates in the search for new optical materials too [1, 2].

In this work structure and optical properties of composites Nd_2O_3–, $Nd_{9.33}Si_6O_{26}$/fumed silica were studied using X-ray diffraction (XRD), scanning electron microscopy (SEM), electron spectroscopy. As the XRD data show phase $Nd_{9.33}Si_6O_{26}$ is formed due to the interaction of neodymium and silicon oxides at temperatures from 920° C for a wide range of oxide ratios (Fig. *a*, *b*). The correspondence of the phase composition to the phase diagram is observed at temperatures around 1400 ° C only.

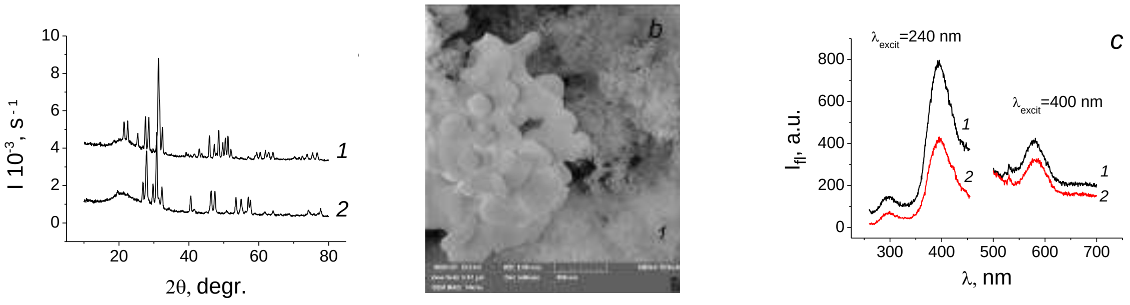

Fig. XRD patterns (*a*), SEM image (*b*), fluorescence spectra (*c*) of the samples:
1 - $Nd_{9.33}Si_6O_{26}/SiO_2$, *2* - Nd_2O_3/SiO_2

It is shown that the composites have similar fluorescence spectra with fluorescence at 400 and 580 nm, excited by radiation with wavelengths of 240 and 400 nm, chosen on basis of absorption spectra of the composites (Fig., *c*).

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Corrosion resistance of nanocomposite electrochemical coatings Ni-Al_2O_3

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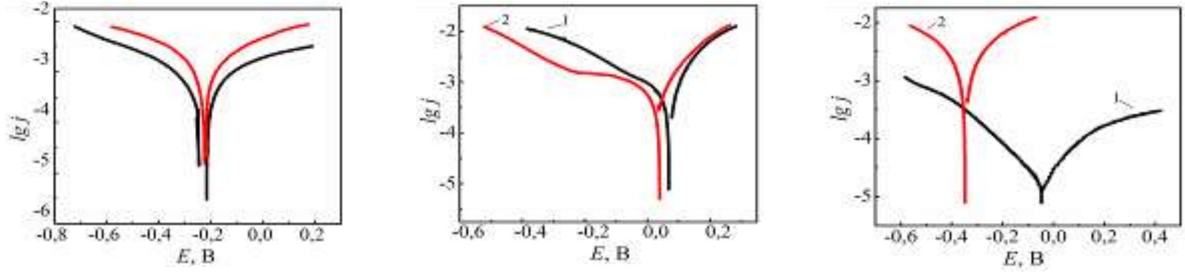
The use of composite materials can significantly increase the strength and characteristics of the product, and the combination of matrix and reinforcing metal components allows to obtain materials with desired properties to optimize the design, taking into account the required characteristics. Strengthening of nickel matrix ultradispersed particles Al_2O_3 leads not only to improve the mechanical properties and heat resistance [1] and the effect on improving corrosion resistance coatings.

Research electrochemical corrosion resistance of composite coatings based on nickel reinforced nanoscale particles of aluminum oxide was performed in solution 0.001 mol/dm^3 sodium hydroxide (pH=11), 0.001 mol/dm^3 sulfuric acid (pH=3) and 3% chloride solution sodium (pH=7) against the background of 1 mol/dm^3 sodium sulfate.



a *b* *c*

Fig. Polarization dependence CEP Ni-Al_2O_3 (*1*) and nickel plating (*2*) in neutral (*a*), acid (*b*) and alkaline (*c*) media

On the basis of cathode and anode polarization dependence experimentally determined corrosion current density and the depth of the corrosion rate indicator k_h both reinforced and monometallic coating. The obtained dependence suggest improving the corrosion resistance of composite coatings compared to monometallic counterparts. Chemical resistance against the composite electrochemical coatings monometallic nickel coatings most significant increases in alkaline medium, which is a reflection of a significant shift in corrosion potential side electropositive values, indicating the nature of the partial inhibition reactions. Probably cause this behavior composite electrochemical coatings structure is more dense sediment, which is consistent with the data of atomic force microscopy.

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Broadening of analyte bands in electroosmotic flow through microchannels with different zeta potentials of walls.
Pre-Taylor asymptotic regime

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The present research is concerned with mathematical modelling of the behaviour of analyte bands transported by electroosmotic flow through slit channels whose walls have different zeta potentials. We conducted simulations of band dynamics in such a flow. According to our results, after a certain characteristic time from the process beginning, the band broadening is well described by the Taylor theory. According to this theory, the rate of broadening is defined by an apparent diffusion (dispersion) coefficient which strongly depends on the mean cross-sectional velocity. The squared variance predicted by using the Taylor approximation is a linear function of the band displacement.

The major focus of present study is the band behavior in the abovementioned flow before the Taylor-Aris regime is established. The simulations demonstrated that, in the pre-Taylor regime, the squared variance non-linearly depends on the band displacement, and, with increasing time, the respective dependencies approach to the linear Taylor behavior, asymptotically. Simultaneously, the solute distribution within the channel cross-section experiences substantial transformations during the pre-Taylor regime: the initially uniform distributions become strongly non-uniform with well expressed maximums or minimums that decrease with time.

Synthesis and properties of $Fe_{3-x}Cr_xO_4$ nanoparticles for high capacity lithium-ion battery anodes

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In commercial lithium-ion battery, graphitic carbon has long been used as the anode material since the first introduction of batteries due to its excellent cycling stability and relatively low cost. Anodes on the basis of magnetite have some advantages comparing with graphitic carbon, the most important advantages are high capacity and power densities of battery. Obtaining such material with demanded charge characteristics is complicated because it is difficult to get material with predetermined Fe stoichiometry and spinel structure. Anode material with average charge potential higher than 1 V (*vs.* Li/Li^+) can´t compete with carbon regardless their capacity due to decrease of power density of battery. The present report devotes to developing of anode materials with high capacity and low charge potential as alternative to commercial carbon material. Polyol method of synthesis of such materials in diethyleneglycol medium with initial precursors $Cr(NO_3)_2 \cdot 9H_2O$ and gluconate Fe(II) has been proposed.

Fe_3O_4, Fe_2CrO_4 and $FeCr_2O_4$ samples with spinel structure and particle size 10-20 nm have been synthesized. In the spinel lattice of Fe_2CrO_4 and $FeCr_2O_4$ samples Cr^{3+} isovalently substitute Fe^{3+}. It is facilitate the decreasing of average charge potential. The samples synthesized show the following charge potentials: 1.75 V (Fe_3O_4), 1.2 V (Fe_2CrO_4), 0.95 V ($FeCr_2O_4$) (*vs.* Li/Li^+). Fe_2CrO_4 material has not Fe^{3+} in its structure, it is the reason why this material has low potential of charge and discharge of material. $FeCr_2O_4$ material during cycling charge/discharge show the stable capacity value of 480 mA h/g.

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Mechanochemical preparation of powder composites with pollen and inorganic carriers

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It is known [1] that mechanochemical grinding of pollen results in getting powders more enriched with biologically active substances (BAS). The increase in BAS amounts during fine grinding associated with cell damage and pollen destruction, as well as the degradation of bonds between biopolymers and low-molecular weight BAS [1] accompanied by an increase in the biological activity of the materials. Addition of inorganic components (silica, coal, clay minerals) provides better mechanical activation and stabilization of low-molecular weight components and biopolymers (vitamins, protein, fiber, pectin).

Highly disperse silica (HDS), clay minerals and activated carbon are used as enterosorbents, so their addition to the composition could provide enhanced therapeutic effect after the release of BAS.

Composite materials have been prepared using inorganic (HDS and clay minerals) and bioorganic (bee pollen) components undergoing mechanical activation performed in a ball mill for 2-3 hours. Relations between components in the composites were changed from 1 : 1 to 1 : 4. For enhanced release of BAS during mechanical activation, 5 ml of 50% ethanol solution was added to the drum.

According to UV spectra, BAS and pollen releasing was stayed. Adding of alcohol solution to the composite material led to increasing the number of components of BAS released from pollen.

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Stimuli-responsive properties of special micellar nanocarriers and their application for delivery of vitamin E and its analogues

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Stimuli-responsive micelles based on di- and triblock copolymers comprised chemically complementary (methoxy)poly(ethylene oxide) and poly(acrylic acid) blocks are used as nanocarriers for encapsulation and delivery in living organisms of poorly soluble in water α-tocopherol acetate (α-TOCA), commonly known as synthetic analogues of Vitamin E.

The self-assembly of asymmetric A-B and A-B-A copolymers with (methoxy)poly(ethylene oxide) (B) and poly(acrylic acid) (A) blocks of a variable length to micelle structures was developed in aqueous solutions at pH<5 by hydrophobic interactions between non-polar bound segments of the copolymer blocks. A different morphology of the given micelle structures (according to an asymmetric character of the block copolymers) and their average particle size were established by TEM images. The presence of complex "core", which stabilized through hydrogen bonds and hydrophobic interactions, give an opportunity of such micelles to show a high binding capability with respect to hydrophobic drugs, in particular to α-TOCA (Fig.).

Fig. TEM images of TBC micelles (*a*) and α-TOCA/TBC micellar mixture (*b*) in aqueous solutions at pH=2.7. φ=0.1 $\text{mol}_{\alpha\text{-TOCA}}$/base-$\text{mol}_{\text{PAAc}}$

Encapsulated α-TOCA provided *in vivo* its full assimilation by animals (white mice), high efficacy through a long-time circulation in their organisms and the reduction in its therapeutic concentration in 25 times.

Physicochemical properties of bimetallic Ag/Cu nanoparticles in bactericidal tissues

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Effective bactericidal fabrics modified with Ag and Cu nanoparticles (NPs) were produced by the developed by us method of soft heat treatment of tissue impregnated with silver and copper ions and characterized by the diffusion-reflectance spectra (DRS), SEM, XRD, electrical resistance and the flame atomic absorption spectroscopy (FAAS) methods. High antimicrobial and antimycotic properties of tissues with low concentrations of Ag and Ag/Cu NPs (in the range 0.06 - 0.25 wt.% for Ag and 0.015-0.13 wt.% for Ag/Cu) are confirmed in experiments with a wide range of multidrug resistant bacteria and fungi: *E. coli, E. aerogenes, P. mirabilis, K. pneumoniae, C. albicans yeasts* and *micromycetes.* XRD and DRS measurements of Ag/tissue and Ag/Cu/tissue samples show the formation of Ag, Ag/Ag_2O, Ag/Cu_2O, Ag/CuO NPs with the size of 20 – 60 nm within cotton. Besides that on the surface of Ag/Cu / tissue insignificant amounts of concurrent compounds such as stromeyerite (CuAgS) and dolerophanite ($Cu_2O(SO_4)$) not possessing bactericidal properties are formed. The FAAS method show the quantitative Cu:Ag ratio as 1:1 within the Ag/Cu/tissue. Dried bactericidal fabric does not have electrical conductivity indicating the absence of contact between particles, fixed in the tissue structure. The electrical resistance of fabrics decreases sharply upon wetting in the water or electrolyte solution suggesting the diffusion of corresponding particles in the tissue and interaction of bactericide agents with microbes in biological fluids. Bimetallic fabrics are the most promising. A basis of cotton - a cellulose is simultaneously the reductant of ions and stabilizer of appearing NPs. C. Pulgarin showed (2010) that CuO reduced to Cu_2O instantly after contact with *E. coli.* Weak visible light results a dramatic increase in inactivation of bacteria because of catalytic character of copper oxide. Obtained composites demonstrated excellent antimicrobial and antimicotic activity even after washing.

Combined acrylic hydrogels-cotton tissues modified with Ag and Cu nanoparticles for medical application

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The subject of this work is the production of effective bactericidal coatings by combining of biocompatible porous hydrogel acrylic films and cotton tissues containing small amounts of nanosized silver and copper particles. Elastic mechanically strong porous acrylic hydrogels selectively adsorb and prolong release a variety of drugs (antibiotics, bactericides, hemostatics, anesthetics, noble metal nanoparticles), can be used to treat burn wounds and promote a normal regeneration process, but sometimes exhibit insufficient mechanical strength. The combination of a hydrogel acrylic film with a bactericidal tissue containing silver and copper NPs leads to additional mechanical strength and a prolonged bactericidal action.

Cotton fabric is impregnated with silver and copper salts in a molar ratio of 1: 1 and thermally treated at 200-220^0 C. Ag NPs and Ag/Cu metal and oxides NPs are formed on the tissue' surface (size 20-60 nm). Then tissues are covered with acrylic hydrogel and dried. The resulting composites show a pronounced antibacterial and antifungal properties over a wide range of pathogenic bacteria and fungi, including *E. coli, P. aeruginosa, E. aerogenes, P. mirabilis, K. pneumoniae, S. aureus,* and others. It should be noted, that uncoated by polymer cotton fabrics have a higher bactericidal activity compared with the same fabric with a layer of hydrogel (zone growth retardation 21-23 and 16-18 mm, respectively). But fabric coated with hydrogel bandage can extend the range of use of wound coverings and improve the process of its regeneration, preventing dry necrosis. The binary composites provide addition strength of the material and allow the use of a relatively thin layer of hydrogel compared to commercially available analogues.

Sorption-desorption of nitrogen on the surface turbostratic graphene-like boron nitride

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The invention of modern industrial sorbents for cleaning water, which can to restore their good characteristics associated with materials based on boron nitride with disordered layers t-BN$_g$. The surface area (BET) 1500 - 1700 m^2/g. Meso- (size> 20 - 50 nm) and macropores (>100 - 200 nm) are forming. Gravimetric capacity to exceeding absorbate (oil pollutions) over the weight of absorbent in the first cycle is to 2899 - 3300% and 1800% in the next five cycles. High sorption properties were detected towards dyes, solvents and heavy metal ions (400 - 600 mg/g). Methods of recovery varied from burning, washing, dissolving to ion exchange with the eluent. The absorption of these substances is in due to own interstitial porosity of the sorbent. It was the subject of this work [1, 2].

Purified examples of t-BN$_g$ were investigated by adsorption-structural static volumetric method on the device ASAP 2000M designed to determine the adsorption isotherms of gases (nitrogen, argon, krypton, and others non-aggressive gases). Measuring range of the method is in the range of pore sizes from 0.3 to 300 nm.

Structure of porosity for boron nitride powders t-BN$_g$ was determined. The material have described as homogenous, micro-mesoporous (monodisperse) with a narrow distribution slit-like pores that is in the range of 3.53 - 4.12 nm, which accounts for about 55% of the volume and 60% of the mesoporous surface. The area of the outer surface of mesoporous is 28.3 m^2/g (t-method) and internal surface - 141 m^2/g (method BJH) [3].

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Direct synthesis of some transition metal lactates

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Recently it has been reported the key role of lactate metabolism in carcinogenesis that can give impetus to the development of new approaches to cancer treatment [1]. In this respect, there is a great need for systematic research on preparation, structure, physical and chemical properties, and biological activity of lactates. The choice of transition elements as metal centres of lactate complexes was caused by their potential application as antitumor drugs [2, 3].

In the work a series of *d*-block metal lactates was obtained *via* "direct synthesis" strategy based on the usage of metals or their oxides as the starting materials [4]. The following systems were investigated:

$M^0 – H_2lact – Solv \rightarrow$ (in air, $t = 60^oC$, magnetical stirring)

where M^0 = Mn, Fe, Co, Ni, Cu, Zn, Cd; H_2lact = lactic acid; Solv = CH_3OH, DMF, DMSO and H_2O.

Yields of products achieved 90% based on metal. Composition and structure of the compounds synthesized were characterized by means of elemental analyses, UV-Vis and IR spectroscopy.

Several of the formation equilibriums were studied by combination of ^{13}C NMR and EPR spectroscopy techniques and the results will be discussed.

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Solubility in thin Cu-Pb and Cu-Bi films

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In the present work, the estimation of solubility of bilayer films has been made in accordance with the data concerning crystal lattice parameters change of components. *In situ* electron diffraction studies were carried out during the Cu-Pb and Cu-Bi films heating directly in the electron microscope column. Samples for the study were prepared by condensing metals from independent sources in a vacuum of 10^{-7} torr. In one experiment the samples of two types were obtained: Cu-Pb films to be studied and reference samples in which copper and lead were separated by a layer of amorphous carbon, excluding their interaction with each other. This made it possible to take into account the influence of thermal expansion on the values of the crystal lattices parameters.

It has been found that in reference films the coefficient of thermal expansion coincides with that one which is typical for massive samples. At the same time, in films in which the studied substances were not isolated from one another, systematic deviations of the lattice parameter of the fusible component from the expected values due to the values of the known thermal expansion coefficient have been observed. This can be explained by the dissolution of copper in the fusible component. The estimation of the solubility value was made by assuming a linear dependence of the crystal lattice parameter (Cu-Pb) and the atomic radius (Cu-Bi) of the fusible component on the dissolved substance.

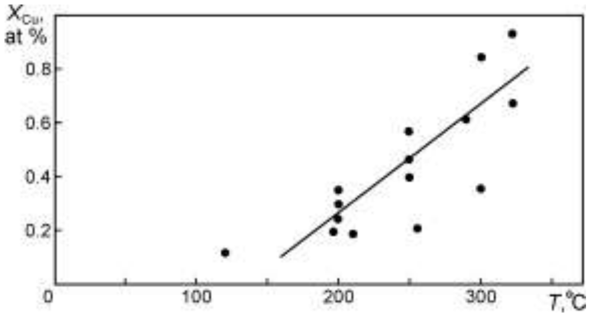

Fig. Dependence of copper solubility in solid lead on temperature in Cu-Pb films

It is seen (Fig.) that the solubility of copper in lead increases with temperature, reaching 0.8 wt.% near the melting point of lead. The value obtained is more than an order of greater than the value known from the literature. The maximum solubility in Cu-Bi films is estimated at 0.9 wt.%, which can no longer be considered negligible, as indicated in the literature.

Thermal dispersion of polycrystalline Cu and Cu-Pb films

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The study of the thermal decay of Cu and Cu-Pb films into individual islands has been performed in this work. Samples were obtained by sequential condensation of metals from independent sources onto an extended alumina ceramic substrate in a vacuum of 10^{-6} torr. The system of moving shields made it possible to produce several films different in the concentration of lead in a single vacuum cycle. Two series of samples were obtained. In the latter, immediately after the condensation along the substrate, a temperature gradient was created, which was maintained for half an hour. In the former, before the gradient was created, samples were annealed at a temperature of 150°C for two hours. The films were then cooled in vacuum to room temperature and examined by SEM. Samples for TEM were deposited on fresh chips of NaCl single crystals, which were heated to the required temperature.

It has been found that a boundary, which according to SEM studies corresponds to the transition from a continuous film to an island film is visually observed on the substrate. The temperature of copper films de-wetting increases with the thickness also for samples 50 nm thick, which were dispersed immediately after the condensation, and it is 365°C. However, the temperature of films de-wetting that were pre-annealed increases and for the films of the same thickness it makes up 490°C. According to TEM studies, this can be explained by an increase in the average size of crystallites composing the film and a corresponding decrease in the proportion of triple junctions and other similar defects, primarily responsible for dispersion. At the same time, the decomposition of Cu-Pb films, when the lead content is greater than 3 wt.% occurs during its melting, regardless of the preliminary annealing.

By SEM studies it has been found that, near the temperature of solid film decay into individual islands, through pores are formed in it, the average size of which increases with temperature. Based on the obtained temperature dependence of the pore size, the activation energy of pore formation is estimated, which in the case of copper films corresponds to the activation energy of surface self-diffusion. It turned out to be 1.6 eV for copper films and altogether 0.2 eV for Cu-Pb films. It should be noted that annealing does not affect the value of the activation energy. The small value of the activation energy of dispersion in Cu-Pb films suggests that their dewetting is due not to diffusion in the solid phase, but to liquid-phase mass transfer.

Microbiological activity of the activated carbon impregnated with silver and selenium nanoparticles

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Activated carbon (AC) is widely used in the pharmaceutical field for the body detoxification and treatment of external wounds. A recent application of AC in clinical medicine is represented by its use in the absorbent material dressings for bandaging the superficial and deep wounds, but also in recovery of post-surgical trauma. These bandages help to create a favorable environment for rapid treatment of wounds and do not allow the spread of infection. AC enhances the process of hemocoagulation, accumulates the exudate on surface, creates a barrier to penetration of microorganisms from the outside and in combination with the dressing material prevents dehydration of the wound. This study was aimed at: impregnating the AC with Enoxil medicinal preparation, as well as Ag or Se nanoparticles, qualitative and quantitative study of the processes to immobilize the neutral nanoparticles on intact and oxidized CA and testing the microbiological activity of the obtained AC samples. Microbiological analyses of the AC samples impregnated with Enoxil preparation and Ag or Se nanoparticles were carried out on Gram-negative *E. coli* bacteria and *Candida albicans* fungus strain.

The AC samples impregnated with nanoparticles have a delayed action on the *E. coli* bacteria, the bactericidal effect being noted only after 4 h for Se and 24 h for Ag nanoparticles, respectively. In the case of *Candida albicans* fungi, for the sample containing Se nanoparticles there has been attested a period, in which the preparation was passive too, but a sharp drop in the number of colonies occurred thereafter. These observations may be explained by the presence of a protective coating the nanoparticles, which do not allow them to aggregate and interact with the atmospheric oxygen, but also prevents the direct contact with the microorganisms. The AC sample impregnated with Enoxil shows bactericidal properties after 4 h in the case of *E. coli* and inhibits growth of *Candida albicans* fungi as well. The activity of the modified AC on *E. coli* bacteria decreases in the series: AC-Enoxil > AC-Se > AC-Ag, while on *Candida albicans* fungi: AC-Ag > AC-Enoxil > AC-Se, correspondingly.

Acknowledgements

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Cathodic reduction of oxygen in the presence of dispersed Fe_3O_4&Ag^0 nanocomposites

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Biomedical application of nanosized materials currently is of increasing interest among all of the world researchers. Magnetic nanoparticles based on Fe_3O_4 are used in various fields of science and technology, such as chemistry, biology, biotechnology, medicine, *etc*.

The aim of this work was to study electrochemical characteristics concerning oxygen reduction on the surface of dispersed Fe_3O_4&Ag^0 nanocomposites formed via so-called rotation-corrosion dispergation procedure, which was described in detail previously [1]. Electrochemical measurements were carried out using a ‘‘floating’’ gas diffusion electrode in an electrochemical cell with separated cathode and anode spaces at 20º C in a 1 mol per l KOH solution using a PI-50-1.1 potentiostat.

Tafel slopes of stationary polarization curves $\partial E/\partial \lg j$ for nanocomposites with Ag^+ content from 0.5 to 5.0 mg/L lie within the limits: b_1 = 0.058-0.057 V, b_2 = 0.101-0.128 V. For nanocomposites with Ag^+ concentrations from 10.0 to 20.0 mg/L those values lie within the limits: b_1 = 0.067-0.090 V, b_2 = 0.122-0.134 V. The largest calculated exchange current ranging $j_0 = 1.7\cdot10^{-2}$ A per g was registered for the nanocomposite {Ag (20.0 mg/L) Fe_3O_4}. The lowest j_0 were observed for nanocomposites with silver content below 10.0 mg/l.

On the basis of electrochemical kinetic calculations of exchange currents and slopes of Tafel curves for the nanodispersed Fe_3O_4&Ag^0 composites, we can conclude that oxygen reduction reaction proceeds mainly through the formation of hydrogen peroxide. The increase in exchange currents due to oxygen reduction reaction for materials with a Ag^+ content of 1.0 and 5.0 mg/L, probably, causes the incorporation of silver into Fe_3O_4 structure. Hence, further increase in Ag^+ concentration during the nanocomposites construction is offset by a larger amount of silver nanoclusters formed on the Fe_3O_4 surface or by a whole shell completion over Fe_3O_4 core, thus forming a core–shell type nanostructure Fe_3O_4 & Ag^0.

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Preparation of thermoplastic starch and biodegradable compositions on their base

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Tradition plasticizers for starch can exhibit substantial drawbacks when used in a preparation of thermoplastic starch (TPS). We have used the eutectic mixture choline chloride (2-hydroxy-N,N,N-trimethylethanaminium chloride) – sorbitol. Because eutectic mixture choline chloride – sorbitol is melting at 25 ^{o}C, the mixing with corn starch is carried out in liquid phase. In the present study, we use maleic anhydride (MAH) as the compatibilizer without and in the presence of dicumyl peroxide (DP). IR-spectra of maleinated starch are presented in Fig. The thermal plasticization of starch and its compatibilizing modification with MAH was accomplished in a duble-screw extruder at 175 °C. In the presence of MAH-DP, the compatibility of thermal plasticized starch / low-density polyethylene (TPS-g-MAH/ LDPE) and TPS-g-MAH / PP blends using MAH as compatibilizer were investigated. It was found that with the addition of MAH, the blends have good interfacial adhesion and finely dispersed TPS and LDPE phases, which is reflected in the mechanical and thermal properties of the blends. The blends containing MAH showed higher tensile strength, elongation at break, and thermal stability than those of blends without MAH. The product in the form of strip is made by single-screw compounding in which a chemical coupling occurs between the starch and LLPE and PP matrix, which accounts for the material's excellent properties. Biopolymer PP-LDPE with TPS-g-MAH as prepared has higher homogeneity, strength, and heat resistance than no-maleinated plastic.

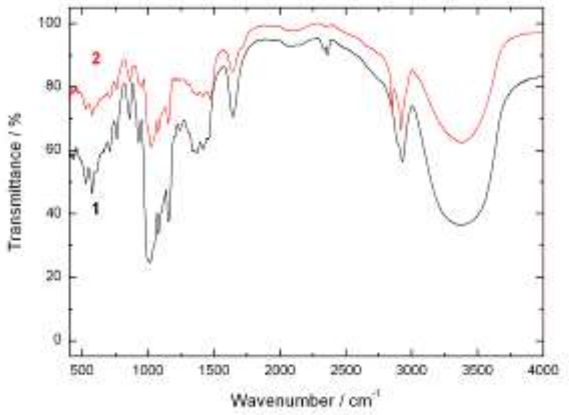

Fig. IR- spectra of maleinated starch: *1* – initial, *2* – with BP addition

New nanoheterostructures: artificial atoms and quasimolecules

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The results of theoretical investigations of excitons states (electron-hole pairs states) in a quasi-zero-dimensional nanosystems (artificial atoms) consisting of spherical semiconductor nanocrystals (quantum dots (QDs)) placed in transparent dielectric and semiconductor matrices. The theory of exciton states in a QDs under conditions of dominating polarization interaction of an electron and a hole with a spherical (QD–dielectric matrix) interface are developed. An shown, that the energy spectrum of heavy hole in the valence band QD is equivalent to the spectrum of hole carrying out oscillator vibrations in the adiabatic electron potential. We show that the absorption and emission edge of QDs (artificial atoms) is formed by two transitions of comparable intensity from different hole size–quantization levels and into a lower electron size–quantization level. Propose a theoretical prospect of using hole transitions between equidistant series of quantum levels observed in nanocrystals for desining a nanolaser [1]. The effect of significantly increasing the exciton binding energy in QDs of ZnSe and Ge, synthesized in a glass and Si matrix, relative to that in a ZnSe and Ge single crystals is revealed [2].

We developed the theory of a exciton quasimolecules formed from spatially separated electrons and holes (the hole is in quantum dot volume, and the electron is localized at the outer surface of the quantum dot–dielectric matrix interface) in a nanosystem that consists of ZnSe and Ge QDs synthesized in a glassy and Si matrix [3].

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Organic-inorganic ion exchangers based on the strongly and weakly acidic polymeric matrices

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The aim of the investigation is a purposeful control of a state of the inorganic constituent in ion exchange polymer. The purpose of the study is also to establish the influence of the particles on the polymer structure and functional properties of the composites.

Organic-inorganic materials based on flexible gel-like strong and weak acid cation exchange resins were obtained by means of its modification with zirconium hydrophosphate. The samples were investigated using transmission and scanning electron microscopy, standard contact porosimetry as well as impedance spectroscopy.

Single nanoparticles (4-10 nm) and their aggregates were found inside the polymer. Evolution of porous structure of the polymer constituent affected by the inorganic particles is considered, the modifier has been shown to decrease the content of free water in the polymer, to increase swelling pressure, which is determined according to Gregor model, and to provide a growth of ion-exchange capacity in a comparison with the pristine resin However, increasing of the modifier amount causes a growth of electrical conductivity of the composites. The ion-exchanger with a maximal content of zirconium phosphate (67 %) was applied to removal of Ni^{2+} and Cd^{2+} ions from a solution containing also hardness ions and organics. The composite provide continuity of the process, the removal degree of toxic ions reaches 96-98%. Redistribution of the nanoparticles in the polymer, which is affected by electric field, has been found.

The modified samples demonstrate improvement of selectivity and higher break-through capacity in a comparison with initial ion-exchange resin. This is caused by inorganic constituent on the one hand and partial exclusion of acidic groups from ion-exchange process on the other hand.

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Nanosilica action on the character of binding water in composite systems with the Enoxil biopreparation

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The extracted, by freeze-drying or vacuuming, components of plant material, microbial preparations or tissue homogenates are very hygroscopic and easily absorb considerable amounts of water being in contact with atmospheric air. An effective way for their stabilization is to generate composite systems with nanosilica. As the bio-preparations in the air can be subjected to bacterial and fungal contamination, nanosilica, linking a large number of microbial bodies, is able to prevent their degradation, increasing the duration of the storage. A promising way case is to find such nanomaterials that reduce the amount of water absorbed by the biological component of the composite material. As a physical basis can serve the transfer of the biological component into nano-sized state where there is no formed bulk organic phase. Within the nanostructured mineral matrix, at a certain ratio of the concentrations of biological and mineral components, the islands of biological component with a size comparable to the one of the interparticle empty spaces of silica, can be formed. Since the solubility of water in the nanoscale biosystems may differ significantly from the bulk one, this effect may be used to reduce their hygroscopicity. The aim of this paper has been to investigate the effect of hydrophilic and hydrophobic nanosilica on the processes of freezing and evaporation of water, linked to the preparation “Enoxil”, and obtained by extraction and chemical treatment of biologically active substances from the grape seed. By low-temperature ^{1}H NMR spectroscopy and thermogravimetry methods, the effect of hydrophobic (AM1) and hydrophilic (A-300) nanosilica on the process of evaporation and freezing water, linked to hygroscopic grape seed extract, bio-preparation Enoxil (Ex) has been studied. It is shown that nanosilica modifies the character of binding water in composite systems. The total amount of water retained in the composite becomes substantially smaller than in pure bio-preparation. It varies in the series Ex> Ex/A-300> Ex/(A-300 + AM1)>Ex/AM1, which is reflected in values of the water absorbed mass, as well as in the values of interfacial energy, concentration of strongly bonded water and the cluster size of the adsorbed water. It is suggested that the observed effect is due to formation of the nanoparticles of bio-preparation, in which the water solubility is substantially less than in the bulk of Ex. This effect can be used to stabilize lyophilized biological tissues and cell cultures.

Synthesis and electrophysical properties of semiconductor heterostructures ZnS/CdS

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Semiconductor nanoparticles have attracted much attention because of their peculiar optical and electronic properties, which have a great potential for many applications. Both CdS and ZnS belong to II-VI group semiconductors, and they have similar crystalline structures. However, ZnS has higher bandgap energy than CdS (3.7 eV versus 2.4 eV when measured in bulk). Due to higher bandgap energy of ZnS, it has been widely used as surface passivating material for CdS.

Heterostructures CdS/ZnS nanorods were synthesized using a two-step solvothermal approach. The first step is the formation of CdS nanorods. Nanorods CdS were synthesized by crystallization of 0.004 M $Cd(NO_3)_2 \cdot 4H_2O$ and 0.008 M thiourea from ethylenediamine $C_2H_4(NH_2)_2$ (30 ml) at 393 K. After cooling to the ambient temperature the precipitate was washed with distilled water, centrifuged and dried at 330 K. The second step leads to the formation of ZnS and further coalescence-exchange leading to deposition and growth of a ZnS particles on CdS nanoparticles. A mixed aqueous solution of zinc acetate and thiourea (1:3 molar ratio) was prepared by stirring for 1 h. The solution was then added dropwise to the CdS solution. The final solution was transferred into a Teflon-lined autoclave and maintained at 433 K for 4 h. The ZnS coated CdS nanorods were centrifuged in water continuously for many times, later dried to obtain the final powdery product.

TEM images of the CdS nanoparticles showing rods with an average length of 150-200 nm and a thickness approximately of 20 nm. Crystalline structure and crystallite size of ZnS/CdS was determined using X-ray method. Diffractograms were recorded on a diffractometer DRON-4-07. Conductivity of the dispersed powder CdS is about $2 \cdot 10^{-5}$ (Ohm cm)$^{-1}$ and the dispersed heterostructures 0.5ZnS/CdS is about $3.5 \cdot 10^{-8}$ (Ohm cm)$^{-1}$. When illuminated mercury vapor lamp of 0.5ZnS/CdS heterostructure the conductivity is an increase of approximately 20%.

Recording diffuse reflectance spectra was carried out on a Lambda-35 spectrophotometer (Perkin-Elmer).

The real (ε') and imaginary (ε'') components of the complex permittivity in microwave range (9 GHz) of the dispersed heterostructures ZnS/CdS is about 2.8 – 4.3 and $6.5 \cdot 10^{-2} – 3.1 \cdot 10^{-1}$, respectively.

Synthesis and electrical properties of ferrites $MeFe_2O_4$ (Me = Ni, Zn, Co)

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The spinel ferrites are an important class of magnetic materials which have been extensively investigated during the past few decades for their potential applications in the fields of biomedicine, environmental remediation, catalysis, spintronics, microwave devices, magnetic storage, magnetic refrigeration devices *etc*. Large-scale applications of ferrites and potential of tailoring of magnetic and electrical properties have prompted the development of several synthesis methods and strategies.

The chemicals used for the preparation of the samples $MeFe_2O_4$ (Me=Ni, Zn, Co) were nitrates: $Co(NO_3)_2{\cdot}6H_2O$, $Ni(NO_3)_2{\cdot}6H_2O$, $Zn(NO_3)_2{\cdot}6H_2O$ and $Fe(NO_3)_3{\cdot}9H_2O$; citric acid (C_6H_8O) and ammonia solution (25%).

$MeFe_2O_4$ (Me=Ni, Zn, Co) were investigated by X-ray analysis (XRD). The real (σ') and imaginary (σ'') components of the complex electrical conductivity ($\sigma^*=\sigma'+i\sigma''$) at low frequencies (0.1, 1 and 10 kHz) were measured using the immittance meter E7-14 by two-contacts method in the temperature 298 K. The real (ε') and imaginary (ε'') components of the complex permittivity in microwave range were measured using the interferometer at a frequency of 9 GHz.

Our identification of the observed diffraction XRD maximums provides evidence for the fact that in the samples $ZnFe_2O_4$ there is a spinel structure. The calculation results indicate that in the disperse samples $ZnFe_2O_4$, $NiFe_2O_4$, $CoFe_2O_4$ the size of crystallite is about 43, 46 and 25 nm, respectively.

The values of the real and imaginary components of the complex magnetic permeability of samples $Ni_xFe_{3-x}O_4$ are μ'= 1.8-2.1 and μ''= 0.4-0.8, and magnetic loss tangent equals 0.2-0.8.

LDI-ToF investigation of carbon catalyst's surface

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Biomass has received considerable attention as a sustainable feedstock that can replace diminishing fossil fuels for the manufacture of a wide variety of specialty chemicals [1]. Solid acid catalysts play a crucial role at different steps of the biomass transformation to chemicals and fuels.

Sulfonated carbons are considered as promising catalysts for transformation of biomass. They can be inexpensively produced by partial carbonization of sulfopolycyclic aromatic hydrocarbons or sulfonation of partially carbonized organic compounds [2–4].

In this communication laser desorption/ionisation time-of-flight (LDI-ToF) mass spectrometry was used to study the surface groups of sulfonated carbon catalyst. Carbon catalyst was prepared by phosphoric acid activation of apricot stones at 400 °C followed by sulfonation with sulfuric acid at 180 °C. LDI-ToF measurements were performed using an Autoflex II LRF 20 Bruker Daltonics instrument (Germany), equipped with a pulsed nitrogen laser of 337 nm, with a pulse width of 3 ns.

LDI-ToF mass spectra in a positive mode revealed, among numerous carbon clusters C_4-C_{27}, the SO_2 and SO_2H fragments with *m/z* 63.9 and 64.9 respectively. Negative mode showed polyphosphate fragments PO_2 and PO_3 with *m/z* 63.0 and 79.2 as in other phosphorus-containing carbons [5]. Fragments of sulfonic group were present as SO (*m/z* 48.0), SOH (*m/z* 49.0), SO_3 (*m/z* 80.2) and SO_3H (*m/z* 81.2). Thermal heat treatment diminished the intensity of sulfonic group fragments. Relative intensities of SO fragment were 1, 0.56 and 0.07 for initial carbon catalyst and heat treated at 400 and 800 °C respectively. For SOH fragment relative intensities were 1, 0.5 and 0.03.

The study showed that LDI-ToF mass spectrometry is a powerful tool for investigation of functionalised carbonaceous materials.

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In vitro activity of Tamoxifen-loaded magnetite nanoparticles against MCF-7 breast cancer

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In recent years, as an alternative and the most promising trend in terms of practical use, priority was given to the works in the field of creating "nanoclinics" – the multilevel magnetosensitive nanocomposites having the complex of functions that are characteristic of nanorobots, including recognition of specific microbiological objects in biological media, targeted delivery of drugs to organs or cells, diagnostics and treatment of diseases at the cellular and genetic levels, adsorption of cells, decomposition products after exposure to the drug or therapeutic hyperthermia, removing them from the body using magnetic fields, *etc.* [1].

Magnetite was conjugated with tamoxifen order to create highly effective anticancer nanocompsoites. Tamoxifen belongs to a class of nonsteroidal triphenylethylene derivatives (Fig.), widely used the treatment for patients with all stages of breast cancer.

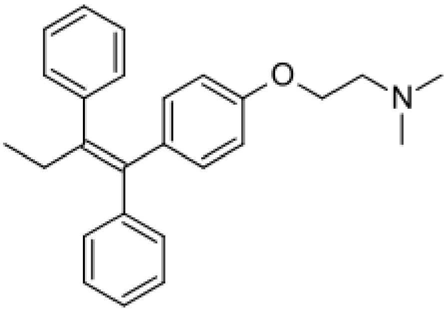

Fig. Tamoxifen chemical structure

Tamoxifen-loaded magnetite nanoparticles stabilized using sodium oleate. Physico-chemical characteristics (TEM, DLS, drug loading *etc*.) as well as *in vitro* activity were investigated.

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Synthesis boron and gadolinium-containing nanostructures

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During last years in the Chuiko Institute of Surface Chemistry magnetosensitive nanocompostites with complex diagnostic and therapeutic functions for biomedical applications have been developed. Created nanocomposites with chemotherapeutic (cisplatin and doxorubicin) agents, contrast agents (CA) and radiosensitizers, antibodies and biocompatible coatings on biopolymers base. Great attention is paid to creation of boron and gadolinium-containing nanocomposites for neutron capture of cancer.

Neutron capture therapy (NCT) is a noninvasive therapeutic modality for treating locally invasive malignant tumors such as primary brain tumors and recurrent head and neck cancer. Neutron Capture Therapy based on the ability of the non-radioactive boron and gadolinium isotopes to capture with a very high probability thermal neutrons.

Methods of synthesis of new Gd- and B-containing magnetosensitive nanocomposites on basis of single-domain magnetite were developed: Fe_3O_4/hydroxyapatite (HA)/Pamidronic acid(PA)/diethylenetriaminepentaacetic acid (DTPA)/gadolinium (DTPA-Gd) (Fe_3O_4/HA/PA/DTPA-Gd^{3+}); Fe_3O_4/aminopropyltriethoxysilane/DTPA-Gd; Fe_3O_4/dimercaptosuccinic acid(DMSA)-Gd; Fe_3O_4/$GdBO_3$; Fe_3O_4/aminopropyltriethoxysilane/furfuryl borate. By FTIR spectroscopy, XRD and X-ray photoelectron spectroscopy composition and structure of the nanocomposites were studied. The synthesized nanocomposites can be used in the fields of medicine and biology, particularly in neutron capture therapy, as a complex of new therapeutic drugs and diagnostic tools for targeted drug delivery accumulation and retention in organs with an external magnetic field.

Acknowledgements

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Adsorption of levofloxacin by glutaraldehyde-crosslinked chitosan-silica cryogels

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Aromatic compounds, such as pharmaceuticals, pesticides and dyes, as well as heavy metal ions, are often found in the industrial and domestic wastewaters. Those compounds are common contaminants of used water and many of them are known to be toxic or carcinogenic. Recently many studies have been focused on the development of sorbents produced from renewable and low-cost raw materials alternative to the traditional synthetic ion exchangers. Materials of biological origin are especially interesting since they are cheap and can be used to remove toxic compounds from various wastewaters.

In current work, cryogels with chitosan-silica of various compositions were synthesized with crosslinking of amino groups of chitosan macromolecules. The influence of the cryogelation on such physicochemical properties as textural characteristics, porosity, morphology of particles, surface structure, and thermal stability of the materials is discussed. It has been found that the cryogels have relatively high adsorption capacity with respect to levofloxacin, fluoroquinolone antibiotic. Thus, one gram of a glutaraldehyde-crosslinked chitosan-silica cryogel could adsorb up to 325 mg of levofloxacin. For the cryogels, the isotherms of antibiotic adsorption from neutral and acidic media were recorded and the values of the constants of the Langmuir and Freundlich models were estimated. The kinetic adsorption characteristics were also studied for the composites. It was shown that the pseudo-second order kinetics is well appropriate (correlation coefficient > 0.99). Theoretical calculations of adsorption capacity were compared to the experimentally obtained values.

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Compatibilization of nanofilled immiscible polymer blends

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Physical-mechanical properties of polymer blends and products from them are primarily determined by thermodynamic compatibility of the components. One of the most effective ways for regulation of the phase morphology is the injection compatibilizers and nanoadditives.

The main aim of this work is to study the impact of nanoadditives and compatibilizers on processes of structurization in the thermodynamically incompatible mixture of polypropylene/co-polyamide (PP/CPA).

The object of the study is a mixture of PP/CPA composition 20/80 wt.%. Multi-walled carbon nanotubes (CNT) brand Graphistrenqth (France) was used as nanoadditives. PP vaccinated with maleic anhydride (PPgMA) was used as compatibilizer in mixtures made up with 2.0 and 3.0 wt.%. Modifiers were injected in PP and then received granules were mixed on single-screw extruder with pre-dried CPA. The kinetics of disintegration of liquid jets (microfiber) in PP matrix with CPA was studied by the method based on dependencies describing thermodynamic equilibrium in disperse systems. Extrudate morphology was evaluated on the microscope by definition of number and size for all types of structures after extraction with PP matrix.

Results of microscopic studies showed that the studied compounds flow-formed matrix fibrillar structure consisting of an isotropic matrix filled with microfibrils component dispersed phase. The injection of CNT and PPgMA in the mixture affects on the patterns of disintegration of liquid jets in PP matrix CPA. The maximum effect is achieved by the simultaneous action of nanoadditives and compatibilizatior: surface tension drops from 2.36 mN/m for the initial mixture to 0.99 mN/m for modified microfibers increases the lifetime for ~ 2 times. The possibility of regulation of matrix-fibrillar extrudate structures of three and four component compositions by improving the compatibility between the components and stability PP microfibers. The process of fiber-fomation in PP matrix with CPA can be improved by using of average diameter of microfibers and the number of films with minimal costs by reducing the formation of new surfaces.

Thus, compatibilization of nanofilled PP/CPA mixtures contributes to the formation of improved matrix-fibrillar morphology due to the synergistic action of modifiers.

Functionalized mesoporous silicas for sorption removal of dyes from aqueous solutions

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The majority of dyes employed in dyeing and printing processes are toxic, carcinogenic and mutagenic compounds. To purify waste streams a lot of treatment technologies are used including flotation, sedimentation, electrochemical processes, photo- and biological degradation as well as sorption extraction. Sorption approaches have been found to be the most popular due to their high efficiency and selectivity.

In the past decades, silica materials with hexagonally ordered mesoporous structure have been studied extensively as potential dye sorbents with high chemical stability, large surface area and pore volume. In the present work, mesoporous silicas of MCM-41 type with chemically attached macrocyclic β-cyclodextrin moieties were successfully prepared by sol-gel condensation of tetraethyl orthosilicate and β-cyclodextrin-silane in the presence of structure directing agent. Implantation of β-cyclodextrin groups into the silica framework was confirmed by the results of IR spectral and chemical analysis of surface layer. Porous structure of obtained materials was characterized by nitrogen adsorption-desorption measurements, powder X-ray diffraction, and transmission electron microscopy.

Analysis of methyl red and alizarin yellow equilibrium sorption data was realized using Langmuir, Freundlich, and Redlich-Peterson isotherm models. Comparison of the coefficients of determination and the reduced Chi-squares obtained from error analysis showed that the Redlich-Peterson isotherm model is the most appropriate for fitting the equilibrium sorption of dyes on surface of both starting and chemically modified with β-cyclodextrin moieties silica materials. It was proved that oligosaccharide macromolecules localized in surface layer of β-CD-containing silica contribute to removing of methyl red and alizarin yellow from neutral aqueous solutions. Synthesized silica materials with immobilized β-cyclodextrin groups have promising potential in sorption, separation and controlled delivery processes.

Textural, structural, diffusional and catalytic properties of Fe_2O_3-Cr_2O_3 system

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The porous material Fe_2O_3-Cr_2O_3 usually employed as catalyst was prepared at several calcination temperature and for several calcination times. The study has been carried out by means of multiple physical-chemical analytical techniques for characterising the materials, but also relied on monitoring and correlating the textural, diffusional, mechanical, crystallographic and catalytic properties. The textural properties indicate intermediate calcination times (1-4 h) and calcination temperatures (723-773 K) to be appropriate; the best catalytic activity is obtained for the samples calcined at 773 K for 1 h, while the crystallographic results limit to maximum 4 h of calcination. The mechanical properties advocate for using a slightly lower calcination temperature than 773 K, while experimental results for BET surface area found the highest value at 746 K (Fig.). Generally, the time of calcination does not affect greatly the diffusional properties, but has significant influence on the textural ones; however, the temperature of calcination has stronger influence upon the diffusional properties. Based on the Knudsen number (*Kn*), diffusion is controlled by Knudsen mechanism, which influences the catalytic activity that increases with the diffusional velocity through a highly porous material characterised by a large surface area and dominated by small pores with radii dimensions below 200 Å.

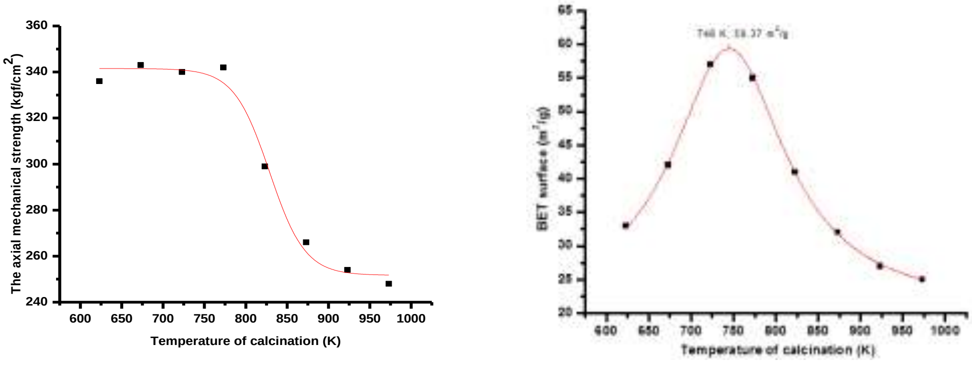

Fig. The dependence on the temperature of calcination of the axial mechanical strength and of the distribution of the BET surface area, after 4 hours of calcination

Physicochemical studies of mechanochemically modified CeO_2-MoO_3 system

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It is known that CeO_2-MoO_3 systems are widely used as catalysts, photocatalysts and catalytic supports [1-3]. Traditional methods of Ce-Mo-O composition preparation such as impregnation, wet mixing, co-precipitation have some drawbacks and the creation of new methods preparation of these compounds is very actual. The alternative method which permits to synthesize complex nanocompositions with larger specific surface area and the structure with specific planes is mechanochemical treatment (MChT).

In this study the mechanochemical treatment in air of the compositions CeO_2-MoO_3=25:75, 50:50 and 75:25 (molar ratio) during 2, 4 and 8 h was performed.

XRD data show that the mechanochemical treatment (independently of treatment duration) of composition Ce/Mo=25:75 leads to a decrease of α-MoO_3 base reflex (020) intensity while the reflex of CeO_2 from the plane (111) becomes basic. At the same time the disappearance of α-MoO_3 reflexes (as a result of its amorphization) for the composition Ce/Mo=50:50 and 75:25 was observed after 2 and 4 h. But an increase of treatment time up to 8 h leads to an appearance of α-MoO_3 reflexes at 2Θ=12.8, 25.7 and 38.9 ° that can be associated with secondary crystallization of molybdena under influence of solid local warming-up as result of treatment. In turn, the MChT accompanied by decrease of initial compounds particles dimensions (from 60 up to 15 nm).

According to the results obtained by BET, it was found that MChT leads to an increase of the specific surface area of the samples from 1 to 11 m^2/g and formation of macro- and meso-porous structure from non-porous initial samples.

Data of TEM show that after treatment the formation of nanorods with the length near 100-300 nm (diameter 30-40 nm) is observed.

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Study of influence of process conditions on adsorption kinetics for 4-nitrophenol on active carbon

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Adsorption methods are widely used in water and waste water treatment technologies [1, 2]. Application of active carbon as an adsorbent allows for effective removal of variety of contaminants, especially organic ones. A special group of toxic substances are aromatic organic compounds such as phenol and its derivatives, pesticides, dyes, pharmaceuticals, surfactants, food preservatives and others. Due to the relatively good solubility of the compounds in question, they can easily migrate into the environment [3-5]. Hence, they require particular attention when optimizing the water and wastewater treatment processes.

The efficiency of adsorption is affected by many factors related to the properties of the adsorbent (specific and external surface area, type and volume of pore, surface charge) and adsorbate (molecular size of the adsorbate, differences in solubility), process conditions (pH), temperature, mixing rate and the presence of other substances [6-7].

The aim of this work was to study of influence of selected process conditions on adsorption kinetics for 4-nitrophenol on active carbon. UV-Vis spectrophotometry applying a flow cell was used for measurements of adsorption rates. The experimental data obtained were analyzed by multiple equations and models of adsorption kinetics.

Acknowledgements
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Preparation and characterization of carbon adsorbents from agricultural wastes

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Adsorption methods applying carbon adsorbents are commonly used in the processes of air, water and wastewater purification. Carbon materials have advantageous mechanical properties and extensive porous structure. Moreover, these adsorbents are non-toxic, cheap in production and easy in utilization [1-3].

One of possible ways of preparation of such materials is carbonization of agricultural wastes (for example: nut shell, fruit seeds, straw, sawdust). Biocarbons (biochars) have a similar or better sorption properties than carbon adsorbents obtained from traditional precursors. Furthermore, in order to improve adsorbing capability for specific compounds, they may be modified, e.g. by removal of ash or impregnation with chemicals [4-7]. Moreover, production of active carbon from waste materials allows the proper management of natural resources and reduce production costs and stress on environment.

The main aims of this study were preparation and characterization of carbon adsorbents from agricultural wastes. Detailed purpose of the study was to determine the suitability of obtained materials as adsorbents for use in water and wastewater treatment by analysis of their properties in such systems.

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

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Features of absorption and emission of laser irradiation by free electrons in ferromagnetic semiconductors

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For today, one of the interesting objects of research are ferromagnetic semiconductors (FMSC), which combine semiconducting and magnetic properties. The presence of strong *s-d* exchange interaction between electronic and magnetic subsystems leads to the fact that in external fields (in particular, in the field of intense laser radiation) conditions implemented to FMN for heating not only charge carriers but also spin waves. It can cause an emergence of periodic patterns of interaction on free charge carriers in electronic subsystem as well as on magnons in the magnetic subsystem. As a result, it can be realized in changing FMSC physical properties in the field of intense laser radiation. First of all, appearance is possible of new conformities in cooperating free carriers of charge with the magnetic subsystem. FMSC can become promising materials for dynamic holography because laser-induced structures such as super-lattices in FMSC have a small relaxation time and a large enough modulation depth. Creating a super-lattice magnetization in FMSC can be used to analyze and control by ultracold neutrons beams [1].

In this paper the features of absorption and emission of light by free electrons in FMSC with laser-induced structures on free carriers are investigated. The general expressions for the absorption coefficient are received in occurrence of hot electrons, also for the intensity of a radiation light by free electrons in ferromagnetic semiconductors (FMSC), which takes into account the dependence on the concentration of electrons, on their temperature and the magnon temperature, for the case when the electron-magnon scattering is dominant. The paper considers classical and quantum cases. It is shown that in the classic range of frequencies when no heating of electrons and magnons takes place, the light absorption coefficient of free electrons in the FMSC differs from the classical Drude formula only by the multiplier. It is established that the intensity of the spontaneous radiation of hot electrons in the FMSC does not depend on the light frequency in the classic frequency range and exponentially decreases in the quantum region of frequencies.

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Composites based on lignin and chemically modified silicas

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Lignin is a multiton waste of the pulp production. This natural polymer determines the mechanical strength of wood. Lignin is not individual substance, but a mixture of biopolymers with different structures typical for various types of wood. All types of lignin are based on phenylpropane units with different substituents. Today the most of lignin is utilized as a solid fuel for power plants, heating boilers, fireplaces, *etc*. Meanwhile, lignin is a valuable chemical raw material using to produce biopolymers, sorbents, and biologically active additives. Unfortunately, the widespread use of lignin as an available raw material for the industry is limited by the properties of this polymer.

Deposition of water-soluble lignin on silica bearing various functional groups by the impregnation method was carried out to study the effect of the biopolymer presence on properties of the obtained composites. Chemically modified fumed silicas with grafted methyl (100 and 30% substitution of surface silanols), silicon hydride, amino groups and their combinations were applied as the carriers.

Composites synthesized have been investigated using differential scanning calorimetry (DSC) analysis. The temperature of glass transition, parameters of structure and morphology of the polymeric layer were determined.

Characteristics of immobilized on the silica surface lignin was found to be different from the properties of the polymer in the volume. The parameters of relaxation and phase transition are determined by structure and functionality of the silica surface layer. Obtained results can be applied for elaboration of the enterosorbents and other nanostructured materials with the desired activity.

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.

Durable carbon sorbents from coal and coke chemical waste

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It was investigated the process and solid products for H_2O-activation (800 ^oC, 30-120 min) of co-carbonisates (1 stage - thermolysis (450-700 ^oC) of blends from long flame coal (D) with coal tar (CT), polymers (P) of benzene separation and coke chemical wastes: fuse (F), sour tar (ST), distillation residue (DR) too. For performance it was chosen surplus coal D (sizes d = 0.5-2.0 mm) with characteristics: W^a 11.1%; A^d 1.8%; V^{daf} 43.8%; elemental composition of organic mass (% ^{daf}): C 80.0; H 5.3; S 1.0; N 1.9; O 11.8.

Using IR spectroscopy it was shown that yet at combining stage chemical interactions between components (coal 85% - waste 15%) take place. Relative intensity of the absorption bands in the region of hydroxyl intermolecular bonds (υ=3400 cm^{-1}) and functional O-containing fragments (υ= 1100-1040 cm^{-1}) in 1.3-2.5 times higher, than same in initial coal spectra. Its values exceed considerably 15%, as it must be at additive behavior of the blends.

At the blends thermolysis (450-700 ^oC) carbonizates yield (52-64%) proportionally related to a density of applied waste. Obtained on first stage carbonizates were activated by water stream at 800 ^OC. Activated carbon (AC) yield depends on blend composition and varies in interval 79 – 90 %. Optimal time of activation is 1-2 h. Specific surface S_{BET} (m^2/g) and total volume V_Σ (cm^3/g) of pores determined on N_2 or CO_2, adsorbed at $p/p_o \sim 1$). Indexes of activation, porous structure expected from CO_2-isotherms, as a rule have more higher value (specific surface - 390-450 m^2/g), than the same from N_2-isotherms. For time activation ≥ 1 h these values are drawn together.

Activated by steam samples with coke chemical waste using have $S_{DFT} \geq$ 500-600 m^2/g, part of micropores consist of 76 – 90 %. At the same time these ACs differ by higher mechanical durability in comparison with AC from alone coal (88-90% against 58%).

Joint conversion coal with coke chemical wastes (carbonization +activation) allows to obtain cheap carbon sorbents with optimal mechanic-sorption properties.

Characterization of chitosan iodide by temperature-programmed desorption mass spectrometry method

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Polysaccharide chitosan, derived from the natural biopolymer chitin, in recent years has proved to be one of the most promising types of biopolymers. The structural, physico-chemical and antibacterial properties of chitosan complexes with iodine are actively studied. The purpose of our work was to obtain the salt of chitosan with iodide acid (chitosan iodide) and characterize it by TPDMS method.

A temperature programmed desorption mass spectrometry apparatus comprising an original high-temperature furnace and a mass spectrometer MX-7304A (SELMI, Ukraine) was used in the work. To obtain chitosan iodide, 300 kDa chitosan and concentrated HI were used. The formation of chitosan iodide goes on in this case according to the following scheme: $(\text{Chitosan-NH}_2)_n + n\text{HI} \rightarrow (\text{Chitosan-NH}_3\text{I})_n$.

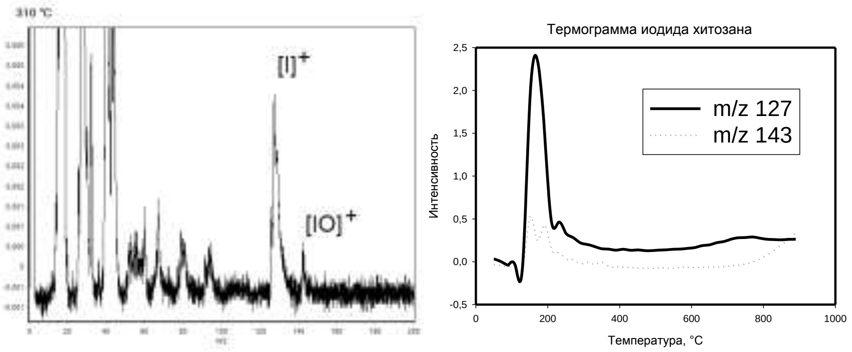

Fig. Mass spectrum for 310 °C (left) and thermograms of I^+ and IO^+ ions (right)

Pyrolysis of chitosan occurs at 290-310 °C. The thermograms show peaks associated with H_2O, CO, CO_2, N_2, I (*m/z* 127), IO (*m/z* 143). The main yield of iodine and the formation of IO occur at 130-180 °C, in step with the breakdown of polymer chains of chitosan. The obtained results indicate the possibility of obtaining iodine preparations in chitosan matrix with enhanced ability of chitosan to retain iodine.

Protolytic properties of mesoporous silica functionalized with diethylphosphatoethyltriethoxysilane

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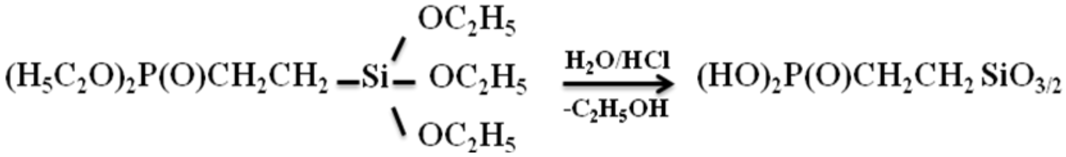
The approaches for the synthesis of mesoporous silica with phosphonic groups in the surface layer have been studied for a long time in our department [1]. The research groups from other countries also study some aspects of the synthesis of the materials, functionalized by diethylphosphatoethyltriethoxysilane (DPTES). That alkoxysilane provided incorporated $P(O)(OC_2H_5)_2$ groups in the silica matrix, which were converted to $-P(O)(OH)_2$ after the hydrolysis of ethoxy groups with the concentrated hydrochloric acid. We also calculated the ionization constants of the hydrolyzed DPTES not fixed on silica matrix (using reaction 1).



$$(H_5C_2O)_2P(O)CH_2CH_2-\underset{\diagdown OC_2H_5}{\overset{\diagup OC_2H_5}{Si}}-OC_2H_5 \xrightarrow[-C_2H_5OH]{H_2O/HCl} (HO)_2P(O)CH_2CH_2SiO_{3/2}$$

(1)

Such groups possess high ability of complex formation with different metal ions. The developed approaches for the synthesis of functionalized silica were displayed on protolytic properties of fixed phosphonic groups. Thus, increasing density of the phosphonic groups per unit of surface reduced the ionization constants. Besides, hydrogen bonds formed between pairs of closely allocated phosphonic groups [2], which also affected the ionization constants. P^{31} NMR spectra identified that the number of such pairs was approximately 10-15% from the introduced phosphonic groups. The calculation of the second ionization constant of $-P(O)(OH)(O)^-$ dissociation had some difficulties because silica network was destroyed in alkaline media.

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Nanocomposites based on graphene materials for the photoelectrochemical systems

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The creation of materials with fundamentally new characteristics is inextricably linked with the production of nanoscale structures. This became possible due to the development of a number of new methods that allow synthesizing structures with properties that are regulated at the atomic-molecular level and unattainable for the structurally homogeneous materials.

We obtained the semiconductor photoelectrodes from the TiO_2 - chalcogenide Cd / reduced graphene oxide (RGO) on a Ti-substrate with formed by us layer of TiO_2 nanotubes. Reduced graphene oxide was received by electrochemical method from the graphene oxide (GO) obtained by the electrochemical oxidation of multi-walled carbon nanotubes [1]. Obtaining GO and RGO by the electrochemical methods was confirmed by electron microscopy, X-ray diffraction, X-ray photoelectron spectroscopy, X-ray emission spectroscopy and Raman spectroscopy.

The photoelectrochemical properties, recombination processes, the surface structure of the nanocomposite films and the heterostructures, as well as their efficiency in photo electrochemical cell (PEC) for the accumulation of hydrogen are studied [2]. It is established that modifying the surface of a semiconductor by V_2O_5 and MoS_x nanoparticles increases the photocatalytic activity of the surface and improves charge separation and prevents recombination processes, which leads to an increase the photopotential and efficiency of the electrode, as well as their effectiveness in photoelectrochemical cell.

It was found that the overvoltage of hydrogen evolution on the cathode of the PEC is gradually decreasing upon transition from carbon nanotubes to anodically oxidized nanotubes and further to electrochemically reduced graphene oxide (ERGO). After the deposition MoS_x to the surface of ERGO and graphene oxide the hydrogen evolution reaction proceeds more efficiently than on smooth platinum and the nickel grid.

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Photo- and electrocatalytic activity of nitrogen-doped iron titanate films

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Doping with nonmetals or metal ions have been employed to tune the electronic structure and enhance the photocatalytic activity of titanium dioxide based materials under both UV and visible light irradiation, improving the efficiency of solar energy utilization.

Herein, we report a simple preparation method of nitrogen-doped TiO_2 and Fe/TiO_2 films, their structure, photoelectrochemical characterization and photocatalytic properties under both UV and visible-light in electrocatalytic reduction of dissolved oxygen and degradation of biogenic (anthropogenic) pollutant – tetracycline hydrochloride as a representative class of antibiotics.

The photoelectrochemical properties of the TiO_2, Fe/TiO_2 and $N/Fe/TiO_2$ electrodes were estimated using the spectral dependence of photocurrent. The films containing iron ions showed lower photocurrent quantum yield than that for undoped samples. Photocurrent quantum yield maximum shifted to the visible spectral range. Iron and nitrogen codoping leads to the anodic shift of the conduction band bottom (ΔE_{cb}) along with the band-gap energy (Eg) decrease. Energy level diagrams of synthesized films were designed by the direct electrochemical measurements that allowed to predict the activity of the semiconductors in the photocatalytic and electrocatalytic processes.

The most significant changes of the flat band potential values were observed for nitrogen contained Ti:Fe=1:1 samples and critically depended on the heat treatment temperatures relating to the formed phase composition. Multicomponent $N/Fe/TiO_2$ films treated at a relatively low temperature (450°C) contain the pseudobrookite structure (Fe_2TiO_5) with landauite ($Fe_2Ti_2O_7$) impurities confirmed by XRD patterns. After treatment at 600°C, the traces of rutile phase appeared. Nitrogen incorporation in the film structure led to the accumulation of iron ions on the surface of the material and acceleration of the $Fe_2Ti_2O_7$ phase formation. High photocatalytic activity of the film under both UV and visible-light irradiation correlated with its high adsorption capacity.

Oxygen reduction polarization curves for TiO_2, N/TiO_2 and $N/Fe/TiO_2$ (600°C) electrodes exhibited single polarographic current wave at potentials of –0.10 to –0.8 V (against SCE) in accordance with energy position of conduction band.

Theoretical investigation of pollutant species adsorption on oxygen vacancies or pure and nitrogen-doped titania

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TiO_2 as a photocatalyst has several advantages due to its high chemical stability, excellent functionality, nontoxicity, and relatively low price, but a serious disadvantage is that only UV light can be used for its photocatalytic capabilities. Only about 3% of the solar spectrum can be utilized due to its wide intrinsic band gap. Therefore, it is of great interest to find ways to extend the absorption wavelength range of TiO_2 into the visible region without decrease of photocatalytic activity.

Fig. Adsorption of water molecules on the N-doped anatase face (001) with an oxygen vacancy

Many techniques have been examined to extend the spectral response of TiO_2 into the visible region and enhance its photocatalytic activity. Impurity doping is one of the typical approaches to extend the spectral response of a wide band gap semiconductor to visible light. Nitrogen incorporation into the lattice structure of titania films was proved by XPS measurements. Quantum chemical calculations were performed to find out the difference between the pure titania and nitrogen doped titania films. The total energy values of the optimized geometrical structures of different size TiO_2 and $TiO_2(N)$ cluster models (including 14 titanium atoms) were calculated using density functional theory m ethod (DFT) and the hybrid B3LYP potential with basis set 6-31G(d,p) by means of the software package PC GAMESS (version FireFly 8.1.0 by A.Granovsky). Clusters were considered simulated for the surface of ideal anatase crystal ($Ti_{14}H_{22}O_{39}$) as well as those for the face (001) with an oxygen vacancy ($Ti_{14}H_{22}O_{38}$) and for the N-doped face (001) with an oxygen vacancy ($Ti_{14}N_2H_{22}O_{36}$).

An analysis of the results of calculations of water adsorption testifies that the adsorption energy on native anatase (-455 kJ/mol) is more preferable than that on nitrogen-doped one (-373 kJ/mol), so insertion of nitrogen atoms into the bulk of anatase crystals results in hydrophobization of its surface.

Synthesis and luminescent properties of hybrid SiO_2 and SiO_2/TiO_2 materials doped with Ln(III) aminopolycarboxylates

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Despite the growing amount of data obtained at silica-containing hybrid systems the interpretation of features of their spectroscopic properties still contradict each other. Some authors claim that the inorganic matrix is not involved in sensitizing the luminescence and the observed increase of luminescent characteristics is caused by reduction of non-radiative pathways, while others propose that there is an energy transfer from singlet and triplet levels of the hybrid matrix to resonant levels of Ln(III) ions. One of the ways to understand the effect of the inorganic matrix is the gradual modification of the hybrid material. In such systems one of the components, silicon dioxide, provides the covalent grafting of the organic compound, while the second component, the lanthanide complex, acts as a luminescent unit. In its turn the inorganic host can be optically «transparent» (SiO_2, Al_2O_3) or optically active (TiO_2, Bi_2O_3). Such methodology leads to hybrids and nanoparticles of different composition, which opens the way for new class materials with unique properties.

In this work, we report the results of spectroscopic studies of Ln(III) complexes with ethylenediaminetetraacetic (EDTA) and diethylenetriamine-pentaacetic (DTPA) acids embeded in silica (Fig.) and mixed silica-titania inorganic matrices. The attachment of Eu(III) complexes was made with the use of both covalent and non-covalent interaction. Peculiarities of the synthesis of such materials and properties of lanthanide-centered luminescence in visible region as well as perspective of practical use are discussed.

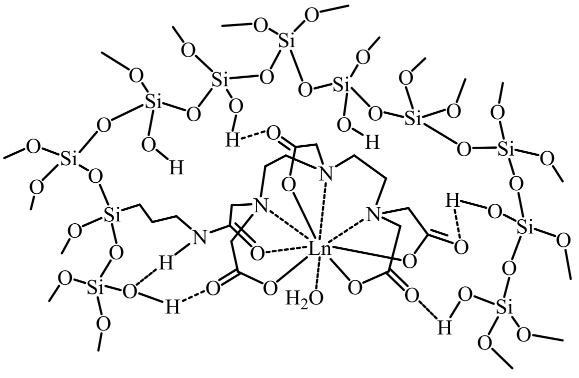

Fig. Example of studied hybrid material with Eu-EDTA complex covalently attached to a SiO_2 network

Diarylethene derivatives for design of downscaled contact electrodes made of Au nanoparticle assemblies

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Development of nano-scaled devices based on gold nanoparticles (AuNP) cross-linked with functional molecules received considerable attention during recent years. Herein we present an approach towards nanoswitches with optically modulated electron conductance. Such switches are a combination of two gold nanoelectrodes (modeled with AuNPs) linked by photochromic diarylethene molecules (DAE). However, developing of nanoswitches requires: (*i*) optimization of molecular structure, (*ii*) stress testing of DAE in contact with gold nanoelectrodes under alternating UV/visible light irradiation, i.e. variance of conductance, (*iii*) development of suitable verification of opto-electronical properties of designed nanodevice.

In contrast to widely used thiophene-based DAE, we use furan based DAE with oxygen instead of sulfur atoms in the photochromic core to suppress binding of molecules via the thiophene sulfur to the Au electrodes. A furan-based DAE showed sub-picosecond ring-closing kinetics under UV light irradiation, outperforming thiophene based switches in ethanol solution. However, in a real circuit an assembly of DAE between gold electrodes is expected to trigger conductance and to operate under ambient conditions. Moreover, in electronic devices scaled to the nano size the occurrence of local plasmon resonance excitation (LSPR) in the Au-electrodes might interfere with the switching process since LSPR is stimulated at the wavelength of visible light which itself induces the formation of the low conductive open-state of DAE.

Cetylpyridinium bromide-modified corn stalks for removal of Acid Red from aqueous solution

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In recent years there is a growing interest in inexpensive and effective adsorbents for the treatment of wastewater containing synthetic dyes. Using of modification natural materials as adsorbent could greatly increase the adsorption of dyes from wastewater. For example, there are numerous studies about cationic surfactant modified clays as effective adsorbents for anionic dyes. Meanwhile, there are only few reports about cationic surfactant modified agricultural wastes (rise husk, coir pith, and barley straw).

In Ukraine corn stalks (CS) are low-cost renewable agricultural wastes. We have chosen cetylpyridinium bromide (CPB) for the modification of corn stalks, because this cationic surfactant shows a high affinity for corn stalks. The modification of CS by the cationic surfactant depends on different factors. However, the study of conditions for obtaining modified CS which coated CPB has never been explored in detail and thus requires investigation.

The objective of this paper is to obtain cetylpyridinium bromide-modified corn stalks (CPB-CS) applicable for the adsorption removal of acid dyes from aqueous solution and to evaluate the influence of such factors as time (τ), temperature (t), weight ratio of CS:CPB (m), and kind of activation of CS (A) on adsorption properties of the adsorbent using full factorial experimental design analysis 2^4. The removal efficiency of Acid Red was dependent response variable.

The full factorial experimental design is a powerful tool to realize the effects of some factors (independent variables) that significantly affect the experimental results. We carried out a factorial design at two levels which included 16 experiments and each experiment was repeated twice.

It was concluded from the full factorial experimental design that: 1) all control factors were significant at the 95 % confidence interval; 2) the influences of control factors decrease in order: $A>m>\tau>T$. The kind of activation of CS, weight ratio of CS:CPB and time have positive effect while the temperature has negative effect.

In this way, it was showed that the optimal CPB-CS (removal efficiency of Acid Red equals 96 %) could be obtained using following conditions: t=20^{o}C, τ=28 h, m=1:0.20, and preliminary activation of CS by NaOH.

Epoxy composites filled with inital and water-hardened inorganic binders (gypsum, cement, chalk)

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The different impact of the initial and pre-cured powders of gypsum and cement on the strength and morphology is filled epoxypolymer (50 wt.%) is experimentally established. The original gypsum and cement in polymer gives the highest modulus in bending, strength of compression (for cement) and micro-hardness than the pre-cured (Fig.). This may indicate activity of the original gypsum and cement in the composition (i.e., the formation of crystals and clusters) that is visible in the photomicrographs (in Fig. *A* and *B* visible crystal-like structure). For both types of chalk a compression strength gave the same result, which naturally indicates the absence of any changes in its structure after water pre-treatment of filler. In general (Table), the introduction of all these fillers leads to a significant (10-20%) higher compression strength, and modulus for flexural strength may increase in 2-3 times.

Table. Strength parameters of the composites with untreated (index "н") and treated water (index "о") with chalk

	Unfilled	Chalk$^{\text{н}}$	Chalk$^{\text{о}}$	Gyps.П$^{\text{н}}$	Gyps.П$^{\text{о}}$	Cement$^{\text{н}}$	Cement$^{\text{о}}$
Compression loading, kgf	510	570	570	560	610	580	510
Compres.Modul., 10^{-4} кgf\cm^2	1.05	1.1	1.1	1.1	1.2		
Micro-hardness, H (for50mcm)	450			420	420	560	500
Flexural Modul., 10^{-3} кgf\cm^2	12.5	22	27	36	21	40	20

A. Unfilled *B*. Chalk *C*. Gyps.Г *D*. Gyps.П *E*. Gyps.C *J*. C-t *K*.C-t hardene

Fig. Micro-image of epoxy-compositions (before the introduction of the hardener) with initial fillers (magnification 400 times). C-t hardened – water-hardened cement

Microscopy shows that the structure of the composites is different for filling the initial and water-hardened gypsum and cement. Fig. clearly shows a changing of the composite morphology after filling. So, chalk is predictable does not introduce any noticeable organized structures in the composition (only the usual seals, Fig., *B*), all taken from the casts were clearly crystalline structure (dendrites, "wolf hair", *etc*., Fig., *C*, *D*, *E*). And cement among other structures also makes a fractals (“snowflake” is visible in Fig., *J*, *K*). Changes in the strength and durability of the composites are explained by the emergence of fractal dendrite structures of gypsum/cement fillers (they are identified microscopically in Fig.) after their water pre-treatment.

Application of organo/layered double hydroxides for the preparation of polyurethane nanocomposites

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The polymer/inorganic composites have received much of current interests as a result of their structure and interesting properties superior to bulk counterparts. The combination of wide applicable polymers with substances of the different chemical nature allows obtaining the new materials with necessary properties. The layered double hydroxides (LDH), one kind of synthetic clay, are used as inorganic nanofillers in the preparation of polymers nanocomposites. The LDH, called as anionic clay, have received considerable attention because of their excellent properties as catalysts, anion exchangers, and biological-carrier materials [1].

Use of LDH in polymer nanocomposites is recently investigated. LDH as nanofiller improves various technical properties (such as mechanical, thermal and barrier) of polymer matrices. Polyurethanes (PU) are one of the most commonly used polymers with a wide range of physical and chemical properties since their morphology and molecular weight can be highly controlled. Polyurethanes are produced by combining diisocyanates with polyols and other chemical additives.

The method of obtaining of organic/inorganic composites based on physical modification of diisocyanates is proposed. Dodecylsulfate (DS) intercalated MgAl LDH were introduced into the polymer matrices. The physical-mechanical properties of synthesized composites contained 0-8 wt.% of DS-MgAl LDH were studied.

Analysis of tensile properties showed significant improvements in tensile strength (TS) and elongation at break (EB) of about 83% and 1185% for PU/DS-LDH (5 wt.%) nanocomposite. The observed excellent concurrent improvement in TS and EB is attributed to the relatively better reinforcing effect of partially exfoliated DS-LDH layers in PU making the present investigation most noteworthy. In addition, gradual improvement in thermal stability with increasing DS-LDH loading makes these nanocomposites versatile and hence suitable for many critical applications.

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The influence of static magnetic field on silica gel free interphase energy

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Magnetic field is one of the most common fields creating the universe. As it was proven before [1, 2], its presence influences some processes taking place in the interfacial area, but investigations consisting influence of static magnetic field on change of values of free surface energy components, according to our knowledge, have never been performed.

The reason of existing all interface phenomena are unbalanced intermolecular forces appearing on the border of two phases and in the layers contacting them, which is was named interfacial tension, or in case where one of the phases is gas – surface tension. Free surface energy or more precisely Gibbs interfacial energy, is function describing the interfacial tension. It can be defined as work needed to create new interface of given area between two phases. Thus, that ability to manipulate its value by applying physical field can revolutionize many areas of human activities.

Basing on van Oss *et al*. approach, components of Gibbs interfacial energy were determined and compared to results of exactly the same experiment carried out without presence of external static magnetic field. Significant differences between experimental results obtained in 0.4 T uniform static magnetic field and outside it suggest that the field presence influences on free interphase energy value of porous silica.

Presented investigations can be useful in topic of the use of magnetic nanoparticles coated by different surface or ligands in different area of science and live.

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Thermal degradation of PDMS-400 filled with initial SiO_2, TiO_2–ZrO_2/SiO_2 and CeO_2–ZrO_2/SiO_2 nanocomposites

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The unusually high thermal and thermo-oxidative stability of polysiloxanes is one of the most important properties of this family of polymers.

The aim of this work was to elucidate the influence of nanofillers (SiO_2, TiO_2–ZrO_2/SiO_2 and CeO_2–ZrO_2/SiO_2) on the temperature conversions of PDMS-400 using thermogravimetry method. The nanocomposites were prepared using a liquid-phase method with the content of grafted CeO_2 and TiO_2 3 (T(C)ZS1) and 10 wt. % (T(C)ZS2) and ZrO_2 10 wt. %. PDMS-400 ($M_W \approx 1700$) was adsorbed onto oxide surfaces in the amounts of 5 – 40 wt. %.

The oxidation and depolymerization are two competing processes which occur during thermo oxidative degradation of the polymer in air. The DTG curves for nanooxide@PDMS samples exhibit three well-defined regions of the mass loss (Fig. 1). The first region is attributed to the removal of physically sorbed water (50 – 120 °C). The second process (180 – 350 °C) is due to depolymerization/oxidation of linear PDMS. In this process three-dimensional cross-linked polymer is formed, as well as chemisorbed polymer on the oxide surface. These polymer structures decompose at 350 – 600 °C. It was determined that the thermal decomposition of PDMS on the surfaces of the mixed oxides begins at lower temperature than in case of initial SiO_2.

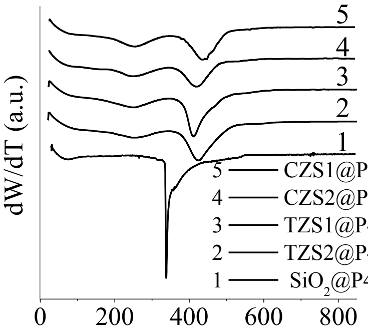

Fig. 1. DTG data for nanooxide@PDMS samples

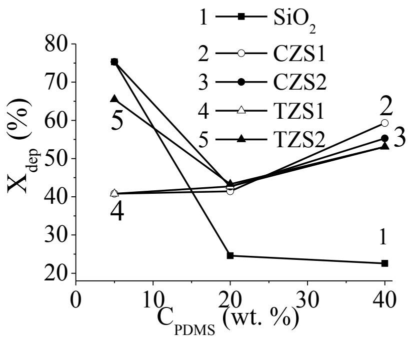

Fig. 2. The degree of transformation of PDMS to SiO_2 and cyclic siloxanes according to data TG analysis

The depolymerisation of the polymer (Fig. 2) dominates for samples SiO_2, CZS2, TZS2 at small C_{PDMS} (5 – 10 wt. %). The presence of titania- and zirconia-ceria on the silica surface promotes the process of depolymerization in the case of more amount of PDMS (20 – 40 wt. %), whereas for initial SiO_2 the oxidation process is more characteristic in this range of concentrations.

Effect of particle size on adsorption activity of biogenic hydroxyapatite towards methylene blue

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It is well known that hydroxyapatite (HA) exhibits excellent bioactivity, biocompatibility and adsorption properties. That is why HA is widely used as adsorbents for controlled proteins and drugs delivery systems. The present study was intended to adsorption activity of methylene blue (as indicator) by biogenic HA (BHA). The effect of particle size was investigated.

The initial powder was BHA Osteoapatyt Keramichnyi® (Ukraine) with different average particle size: ≤ 160, 160-250, 250-500, 500-630 μm. Saturation of BHA performed according GOST 4453-74 using a water solution of methylene blue with a concentration of 1500 mg/l. BHA powder was immersed into the solution for 45 min (250 ml of the solution per 1g of the powder) and than was centrifugated (CLK-1, Russia). The methylene blue concentration on the BHA was determined by photometric analysis (FEK-56M, Russia).

Figure demonstrates the adsorption activity of methylene blue by BHA.

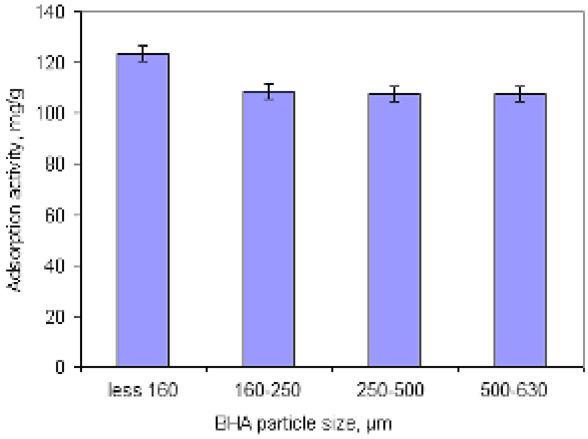

Fig. Adsorption activity of methylene blue by BHA

It was established that the best adsorption activity show BHA with average particle size ≤ 160μm that connected with the highest specific surface area for this powder.

Cu- and Co-containing active carbons as photocatalysts for rhodamine B degradation

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Active carbons (AC) are universal and effective adsorbents for removal organic and inorganic pollutants from gaseous and liquid phases. Besides, oxidized AC possess excellent cation-exchange properties. In recent years, several studies devoted to photocatalytic properties of AC also have been published [1-3]. It was shown that AC containing a heteroatom and surface oxygen groups demonstrate activity in processes of photodegradation of dyes and phenol under UV- and even visible irradiation.

We used oxidized AC and its ion-exchange forms for photocatalytic degradation of rhodanine B (RhB) in neutral aqueous medium. Commercial coconut-shell AC Aquacarb 607C (Chemviron) was oxidized with nitric acid. It has cation exchange capacity 1.8 mmol/g, specific surface area S=1049 m^2/g, total pore volume 0.45 cm^3/g, micropore volume 0.37 cm^3/g. Cu- and Co-doped carbons were prepared by impregnating of oxidized carbon with nitrates solutions, following washing with distilled water and drying. Since AC has a high specific surface area and adsorption capacity, it exhibits photocatalytic activity when its concentration in the reaction mixture is an order of magnitude lower than for conventional oxide photocatalysts, namely 0.1 g/L. Initial AC has no photocatalytic activity under visible illumination but exhibits noticeable activity in UV-region. However, AC improves the photocatalytic properties after introduction of Cu^{2+} and Co^{2+} cations: the rate constant of RhB degradation K_d increases from 1.8 to $2.9 \cdot 10^{-4}$ s^{-1}. The improvement of activity for Cu- and Co-containing active carbons in visible region is even more important: K_d=0.5-$1.2 \cdot 10^{-4}$ s^{-1}. The degree of RhB decolorization for these catalysts is 90% for 3 h but mineralization is only 73% (according to TOC measurements). FTIR spectra of spent photocatalysts also confirm the RhB degradation.

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Effect of SiO_2 dielectric film on the properties of Ge quantum dots

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Epitaxial germanium films on a pure Si(001) surface are widely used as building blocks for modern microelectronic devices. However, further miniaturization of the latter has stimulated the development of integrated structures that include an insulating layer (often made of amorphous SiO_2) between germanium islands and conducting silicon support.

We have considered three structures that differ from each other by a number of Ge atoms and a way of their interaction. Our calculations have shown the binding energy of the first Ge atom with the SiO_2 film to be 6.2 eV, while that for the second Ge atom reduces to 3.9 eV (per adsorbed atom). As far as a dimer Ge_2 is formed on the surface of the insulating film, its binding energy reaches 10.6 eV that stabilizes the entire system.

To clarify the role of the SiO_2 film on the surface of the silicon single-electron density was calculated number of clusters of states: Si/SiO_2, (Si/SiO_2)•Ge, (Si/SiO_2)•Ge_2 and (Si/SiO_2)•2Ge.

To summarize, calculations shifts of core levels the energy in atomic adsorption complexes and Ge dimer on the film of oxidized crystalline silicon at different relative positions of germanium atoms in the surface layer and the results of their comparison with the same range of molecules Ge_2 led to the conclusions: - atomic orbitals completely filled d - subshell germanium atoms taking involved in the formation of internal molecular orbitals that can cause the high surface energy of binding dimer germanium.

Comparative study of benzene and phenol adsorption on mesoporous silicas with various degree of modification

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Benzene and its derivatives are flammable, toxic, carcinogenic and/or mutagenic industrial pollutants, which can contaminate the aquatic environment and drinking water because of theirs high volatility, spreading, and low biodegradability [1]. Among a variety of chemical and physical methods for removal of organic compounds from water, adsorption is one of the most often used and effective approaches. Aromatics is a common chemical compounds, which apply to study the elimination of contaminants from aqueous solutions on different adsorbent types (activated carbon, zeolites, silicas, bio-materials) [2].

In this research, we compare sorption properties of several mesoporous silicas with covalently attached oligosaccharide moieties towards benzene and phenol. Three types of β-cyclodextrin(CD)-containing silicas (β-CD-Silicas) were synthesized by hydrothermal co-condensation of tetraethyl orthosilicate and various oligosaccharide-silanes in the presence of cetyltrimethylammonium bromide. Obtained adsorbents were characterized by FT-IR spectroscopy, chemical analysis, X-ray diffraction, transmission electron microscopy, and low-temperature adsorption-desorption of nitrogen. Their structural properties summarized in Table.

Adsorbent	S_{BET}, **m^2/g**	V_{total}, **cm^3/g**	D_{DFT}, **nm**	**Functional group content, μmol/m^2**	
				[–(CH$_2$)$_3$]NH$_2$	**[β-CD]**
β-CD-Silica-1	812	1.06	3.9; 5.1	0.06	0.02
β-CD-Silica-2	512	0.60	2.5;3.3; 5.1	0.21	0.14
β-CD-Silica-3	457	0.69	2.4;3.1; 4.7	0.26	0.21

Adsorption of benzene and phenol from aqueous solutions onto the surface of MCM-41, aminopropyl-MCM-41 and β-CD-Silicas was studied as a function of time and equilibrium concentration. Experimental kinetic curves were compared with theoretical models of pseudo-first and pseudo-second order processes. Langmuir, Freundlich and Redlich-Peterson isotherm models were used to evaluate adsorption processes and parameters. The higher adsorption performance of β-CD-Silicas towards benzene in comparison with phenol was shown, that may be applicable in the separation of aromatic compounds.

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Clinoptilolite-enriched with phosphate anions at the nanoscale

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Natural zeolites represent nanoporous crystalline hydrated aluminosilicates, tetrahedral of which compose long chains. The structure of their crystal lattice contains voids, which are occupied by freely moving ions and water molecules. After nano-modification (thermal or chemical treatment), the long chains of the aluminosilicate structure can be broken.At the same time, free-moving ions and water molecules are being released from the pores of the zeolite.As a result, it is possible that the structure of the zeolite, its porosity and surface volume changes.This is also accompanied by a change in the dimensions of nanopores of the zeolite or the formation of new nanopores.

In the presented work clinoptilolite enriched with phosphorus was prepared.For this purpose clinoptilolite-containing tuff obtained from Dzegvi (Eastern Georgia) region, with the content of a main mineral composition in the range of 75-85%, was mixed with ammonium dihydrogen phosphate.The material obtained this way retains the structure that characterizes zeolite and also contains ammonium, potassium and phosphate as exchange ions.The cation composition of the used clinoptilote contained mainly cations of calcium, sodium and potassium.Entering an amorphous mass of salt into the structure of clinoptilolite at the nanoscale causes a certain deformation of its structure.

During the nano-modification desorption of water from the zeolite channels, as well as the migration of cations occurs. Ammonium dihydrogen phosphate molecules occupy their place in channels. The penetration of salt into the zeolite structure is indicated by the availability of additional bands on the diffractogram of the melt, which are characteristic of dihydrogen phosphate.In addition, in the IR spectrum of the sample melt, additional bands also appear, which are characteristic for P=O- and P-O-P-bonds in the region of both deformation and stretching vibrations.All of this causes changes in the structure of the zeolite at the nanoscale, although the main microporous structure of clinoptilolite remains. This is shown in the results of the research.

A binding of water by cellulose matrix of medicinal plants and nanosilica (on the sample of *Hibiscus sabdariffa*)

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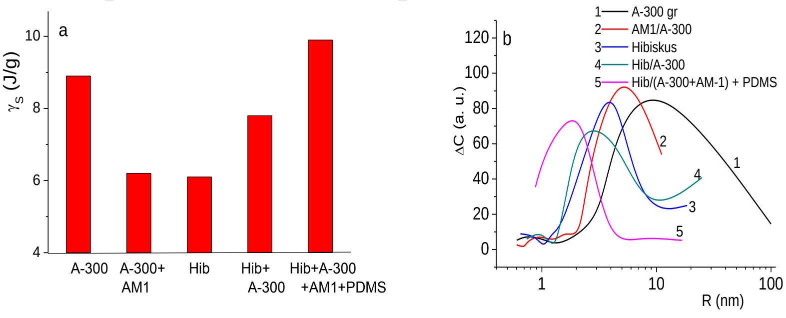
The composite systems based on nanosilica and crushed plants are one of the promising directions for a creating of new types of medicines due to the fact that nanosilica increases significantly water binding. It can be used to produce sustained-release drugs. Besides, nanosilicas due to an interaction with the components of mucosa can create layers of weakly associated water in a contact zone. These layers promote absorption of biologically active poor-water soluble substances with following increasing of bioavailability.

The aim of the present study was to investigate an impact of hydrophilic and hydrophobic silicas on a hydratation of cellulose particles in a model composite system created by mechanochemical treatment of crushed hibiscus flowers and a mixture of nanosilicas.

The low-temperature ^{1}H NMR spectroscopy method was used to study a binding of water in the composite systems based on the both hydrophilic and hydrophobic nanosilicas with dispersed hibiscus flowers. It was shown that for a mixture of hydrophobic and hydrophilic silicas (with a ration 1:1) a reduction in both hydrophilic properties and the radius of clusters of adsorbed water are simultaneously observed, probably due to the formation of narrower gaps between the particles in the composite.



a b

Fig. A diagram of a change of an interfacial energy (*a*) and adsorbed water radii clusters distribution (IPSD) depend on a composition of the composite system (*b*)

It was found, that in the composite systems based dispersed plants and nanosilicas an increase in a water binding energy occurs due to a reduction in a radius of their clusters. This effect is especially strongly expressed in the composites containing hydrophobic silica with adsorbed polydimethylsiloxane. This effect can be used to control a release rate of biologically active substances and for creating of the herbal medicines with prolonged activity and enhanced bioavailability as well.

Natural polymers as adsorbents and flocculants

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Natural polymers are widely used for the efficient phase separation in various technological processes of water treatment, biotechnology, medicine and pharmacy [1]. These are may be natural polymers chitin, chitosan, alginic acid salts. They have a complex of physicochemical properties: biodegradability, reaction and complexing ability, compatibility with living tissues without toxicity.

The researches are devoted to studying adsorption and flocculation activity of natural polymers chitosan and alginic acid salts in aqueous solutions. Chitosan that obtained from shells of crustacean was used as adsorbent. The adsorbent crushed by using a mono-mill. The fraction with the size of particles $(0.2\text{-}0.6)\cdot 10^{-5}$ m was selected for researches. The equations of Langmuir, Hill – De Boer, BET were used for the description of surfactants adsorption. Our researches have shown that surfactants quite good adsorbed by natural polymers [2]. The adsorption isotherms of anionic surfactants concerned to L-type, isotherms of cationic surfactants adsorption - to S-type according to Gilles classification. The results of IR-spectroscopic research of samples of adsorbents and surfactants confirmed there was no chemical interaction in the researched systems in the process of the adsorption. The formation of the hydrogen bonds between the functional groups of chitosan and surfactants is observed.

Flocculation ability chitosan and alginic acid salts were studied in suspensions of kaolin. It was shown, that floculants are more effective in dilute suspensions. The flocculation causes either because of the formation of polymer "bridges", or because of neutralization of the surface charge of the particles. Increasing the sodium alginate concentration leads to a dramatic stabilization system. The most efficient flocculation process suspension occurs when using mixed flocculants. 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.

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Acid-base catalysts based on carbon fibers

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Activated carbon fibers (CFs) are promising materials for the preparation of acid-base catalysts. Chlorination of CFs with CCl_4 and the substitution of grafted chlorine- for S-containing groups are in the focus of this work.

Commercially available carbon fibers *Busofit* (Bus) were used as starting materials to prepared SO_3H-containing samples. Chlorination of carbon fibers was carried out using CCl_4 vapor in argon flow at 450 °C for 2 h. The chlorinated samples (Bus/CCl_4) were treated with concentrated solutions of sodium mercaptoacetate (MA) or sulfide (Na_2S) for the substitution of chlorine with S-containing groups. The same was done with non-chlorinated CFs. Obtained samples were treated with 10% HCl to convert surface groups into the H-form, then they were washed with distilled water and treated with 30% H_2O_2. This caused the oxidation of the surface S-containing groups forming SO_3H groups. The samples were washed with distilled water to a neutral pH of the wash water and dried in air at 120 °C.

The catalytic activity of SO_3H-containing CFs was tested in a model gas-phase reaction of the propan-2-ol dehydration. Analysis of the temperature dependences for the propan-2-ol conversion to propene over obtained catalysts (Figure) shows that the catalytic activities for Bus/CCl_4/Na_2S and Bus/CCl_4/MA are higher than that for non-pre-chlorinated CFs. The temperature of 100% conversion for Bus/CCl_4/Na_2S and Bus/CCl_4/MA is 215 and 220 °C, respectively.

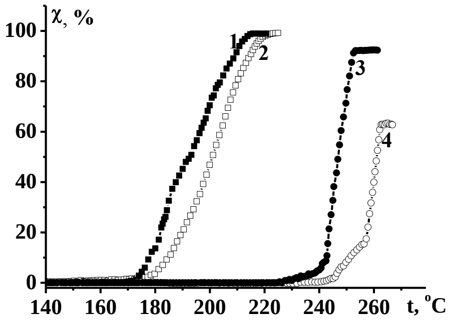

Fig. Conversion of propane-2-ol to propene with the temperature in presence of SO_3H-functionalized CFs: *1* – Bus/CCl_4/Na_2S, *2* - Bus/CCl_4/MA, *3* - Bus/Na_2S, *4* - Bus/MA

Materials functionalized with SO_3H-groups are thermally stable and can be used in acid-base catalysis. Pre-chlorination increases the catalytic activity and the catalysts remain active even after repeated use.

Structure-property relationships for cyanate ester resin/POSS nanocomposites with dual nanoheterogeneity

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Thermostable nanocomposites based on densely cross-linked Cyanate Ester Resins (CER) derived from Bisphenol E and chemically doped by 0.025-1.0 wt.% epoxycyclohexyl-functionalized polyhedral oligomeric silsesquioxane (ECH-POSS), were synthesized in the presence of 20 wt.% $[C_{12}C_6Im][BF_4]$ ionic liquid (IL) and the nanoporous films were obtained by a simple extraction of IL after complete formation of crosslinked CER/POSS network. Recently [1], it was revealed that ultra-low contents of POSS (<< 1 wt.%), covalently embedded into CER network, substantially improved thermal properties and moduli of the latter.

The morphology and porous structure of CER/ECH-POSS nanocomposites developed were confirmed by SEM and DSC-based thermoporometry techniques. The dual nanoheterogeneity of the materials developed has appeared from well dispersed POSS nanoparticles (1-3 nm) and well distributed pores with average diameters in the range of ≈ 45-100 nm and ≈ 20-150 nm, respectively, depending on the POSS content (cf. Fig.).

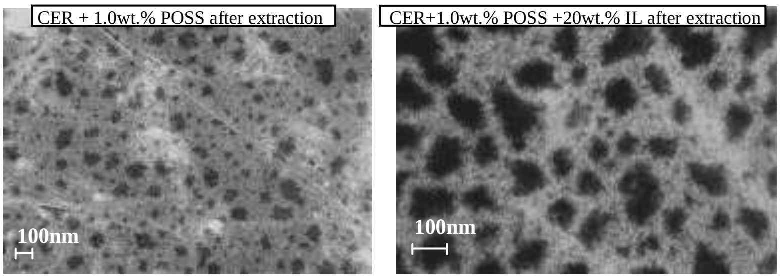

Fig. Typical SEM micrographs of the nanoporous CER/POSS nanocomposites

Acknowledgements

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Justification efficacy of nanocomposite mesh implants for treatment of abdominal hernias

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Treatment of abdominal hernias remains one of the most pressing problems of modern surgery. Generally accepted method of hernioplastic is a tissue plastic using polypropylene (PP) mesh implants. Use of modern implants in surgical practice hasn't quite satisfying effect due to the large number of complications. Therefore, the development of new types of hernia plastic mesh implants remains an urgent problem. We have developed new types of PP allograft modified by carbon nanotubes with antiseptics and modified PP with silver nanoparticles.

The aim of the study was to prove the efficacy of nanocomposite mesh implants for treatment of abdominal hernias.

Comparative evaluation of properties of PP classical implants and new implant research includes mechanical, physical, chemical and antimicrobial properties, the ability to be sterilized by various methods. The reaction of tissues on implantation classic mesh implants of PP and designed implants in rats conducted in compliance with international law and laws of Ukraine on biomedical experiments. The resulting data was subjected to statistical analysis with the definition of reliability differences in different groups of experiments.

Conducted research had shown that modified allograft with nanocomposites and antiseptics is better by physical, chemical and mechanical properties than known PP allografts. In addition, it had shown high antimicrobial activity and good sterilization by different methods without losing its properties. Comparative assessment of morphological changes in the tissues with implantation of PP allograft and modified PP allograft with nanocomposites and antiseptics had shown high biocompatibility of developed allograft. The inflammatory tissue reaction to their implantation was less pronounced compared to the reaction of tissues on the classic mesh implants of PP. Due to this around them had been formed thin connective tissue capsule more earlier than during use allografts from classic PP.

Modification of PP with carbon nanotubes, silver nanoparticles and antiseptics allowed to get new types of allografts, which were characterized by high strength, antimicrobial properties and high biocompatibility. The developed material will reduce the number of postoperative complications and improve outcomes of abdominal hernias.

Efficiency of using the drug based on silica nanoparticles in complex treatment of community-acquired pneumonia in patients with immunosuppression

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The problem of community-acquired pneumonia (CAP) treatment is one of the most urgent problems of modern medicine. Despite the introduction of modern methods of treatment mortality still on the high level, what requires the development of new approaches to the treatment of this disease. We have developed a method of CAP treatment that includes use of an antimicrobial treatment, immunomodulating drugs and enterosorption with nanoparticle silica.

The aim of the study was evaluate the effectiveness of community-acquired pneumonia treatment by the developed method.

Evaluatione of the effectiveness of the developed method was conducted in 79 patients with CAP and immunosuppression, which were divided into two groups: study group (39 patients) and comparison group (40 patients). Both groups of patients were representative by age, sex and comorbidities. In the comparison group, patients received traditional therapy according to the Ministry of Health of Ukraine recomendation, and in the study group additionally was held enterosorption with nanoparticle silica. Evaluation of treatment efficacy was performed by clinical, laboratory, microbiology methods and methods of determining endogenous intoxication. The results of investigation were subjected to statistical analysis and were compared in both groups of patients.

Studies have shown that patients who were treated by developed method was more congenial, because of faster normalization of laboratory parameters of endogenous intoxication indicators and clinical indicators. However, the number of complications such as pleurisy, lung abscess and sepsis patients in the main group was significantly lower. Using the developed method of treatment in patients with immunosuppression possible to reduce the time of patients hospitalization, reduce the number of complications and mortality.

Use of the drug based on nanodispersed silica in treatment of CAP in patients with immunosuppression can significantly improve the results of treatment of this pathology.

Mono- and bimetallic nanoparticles of silver and gold for cancer treatment

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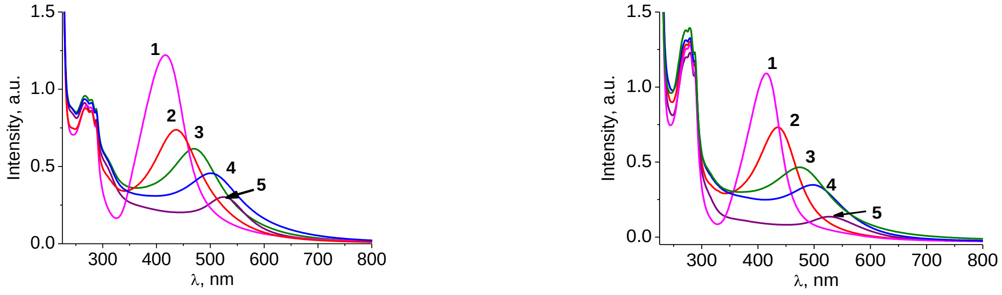
Gold and silver nanoparticles (NPs) can be applied in medicine for targeting, imaging and therapy. The bimetallic composition AgAu could act more effectively in comparison with monometallic NPs, including cancer treatment, due to synergetic effect. Also, the toxicity of bimetallic NPs can be greatly decreased through the use of essential amino acid as reducing and stabilizing agent [1]. Here we used tryptophan (Trp) for reduction of metal ions and also for stabilization of NPs in the colloid according to the procedure developed in [2].

The amount of reducing agent significantly influences the process of particle formation and further growth. In this work we synthesized stable mono- and bimetallic nanoparticles using components in molar amount Trp:M = 1:1 (*a*) and 2:1 (*b*). The influence of tryptophan content on the properties of obtained colloidal solutions was investigated. The optical spectra, zeta potential of nanoparticles and acidity of colloids were discussed. The molar excess of amino acid caused the smaller particle formation, as well as increased their stability. In this case the localized surface plasmon resonance bands in absorption spectra of NPs with predominance of silver were more narrow and symmetrical (Fig.), indicating less intensive aggregation process, that is confirmed by the increased value of zeta potential. For both cases pH of resulting colloids was 8-9. Obtained nanocomposites demonstrated a pronounced antitumor effect when used as “chemotherapeutic agents”.



(a) (b)

Fig. Absorption spectra of colloidal solutions of silver/gold nanoparticles obtained in the presence of tryptophan as reducing and stabilizing agent with components used in molar ratio of Trp:Me = 1:1 (*a*) and 2:1 (*b*): *1* – Ag, *2* – AgAu(3:1), *3* – AgAu(1:1), *4* – AgAu(1:3), *5* – Au

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The employment of filamentous fungus for high-porous surface formations of biocompatible substances

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Compounds based on biocompatible substances are promising materials for implants, absorbers and micromoulds in medicine. The high-porous formations of calcium acetate are the structures with good prospects for manufacture of bioceramics. The mycelium of fungus is example of the natural micro- and nanostructures [1]. Hence, the employment of mycelium as filamentous microstructural substratum for synthesis of high-dispersed systems is a very perspective proposition.

We report in this work the possible employment of the mycelium of fungus for high-porous surface formations of biocompatible substances as calcium acetate. The purpose of this work was to investigate the calcium acetate surface formations. The high-porous surface formations were created by condensation of the volatile molecules of calcium acetate on the mycelium of fungus in the process of vegetative development under the near room temperature conditions. Then the surfaces were observed by optical microscope.

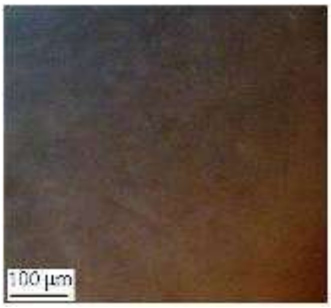

Fig. Image of the porous surface of calcium acetate

From the observations follows that the pores in the calcium acetate surfaces have been of the different size from 1 to 100 μm. Different temperature conditions opens the possibility of changing of porousness. Experiment shows that the employment of mycelium of fungus as filamentous substratum for condensation of the high-porous formations of calcium acetate (Fig.), which are synthesized from a saturated vapour of the volatile molecules, can to change of porousness of the simples and to vary the used in different spheres.

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Synthesis and characterization of Cu-loaded hydroxyapatite-alginate microspheres

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Microspheres of HA in alginate (Alg) shell could be successfully used for controlled release of drugs, growth factors and antibacterial compounds. Hydroxyapatite (HA) is a perfect material for biomaterials production due to its high sorption capacity to metal ions, low solubility in water, high stability to oxidisers and reducers, low cost and biocompatibility [1].

Obtained HA was washed out three times with distilled water and filtered. HA slurry was mixed with 1 and 3% SA solution in ratio 1:1 (samples 1 and 2 respectively). Two ways of synthesis are proposed: 1) HA-Alg mixture was added dropwise into 0.1 M $CaCl_2$ solution, washed out and immersed into 0.1 M $CuSO_4$ solution for 24 h (samples 1f, 2f) (Fig., *a*); 2) HA-Alg mixture was added dropwise into 0.1 M $CuSO_4$ solution for 24 h (samples 1e, 2e) (Fig., *b*).

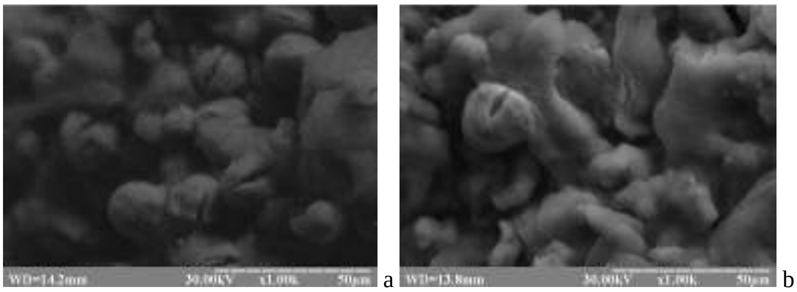

Fig. HA-Alg microspheres obtained in $CaCl_2$ solution and immersed into 0.1 M $CuSO_4$ solution (2 f), HA-Alg microspheres obtained in 0.1 M $CuSO_4$ solution

After 24 hours of microspheres immersion the solution was filtered and concentrations of Cu^{2+} ions in the filtrate were determined by Atomic Adsorption Spectrometry (AAS) method. For samples 1f and 2f filtrate concentrations were the same 0.024 mol/L. In the case of samples 1e and 2e they were 0.019 and 0.021 mol/L respectively. So Alg shell did not have sufficient contribution to adsorption capacity of obtained microspheres.

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The study of thermal decomposition of carbonate apatites by the temperature-programmed desorption mass spectrometry technique (TPD-MS)

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Carbonate substituted apatites (CHA) are widely used as a main components of materials for bone substitution [1]. Samples of CHA $Ca_9Na(PO_4)_5(CO_3)(OH)_2$ (3b), $Ca_{10}(PO_4)_6(OH)_2$ (5b) and CO_2 sorbent material “molecular sieve” (Zeolite X13 60/80) were characterized by using Temperature-programmed Desorption Mass-Spectrometry technique (TPD-MS) [2]. Qualitative and quantitative characteristics of the release of gaseous products produced by destruction of solid-phase samples of apatites under heating (300-1000º) were obtained (Fig.).

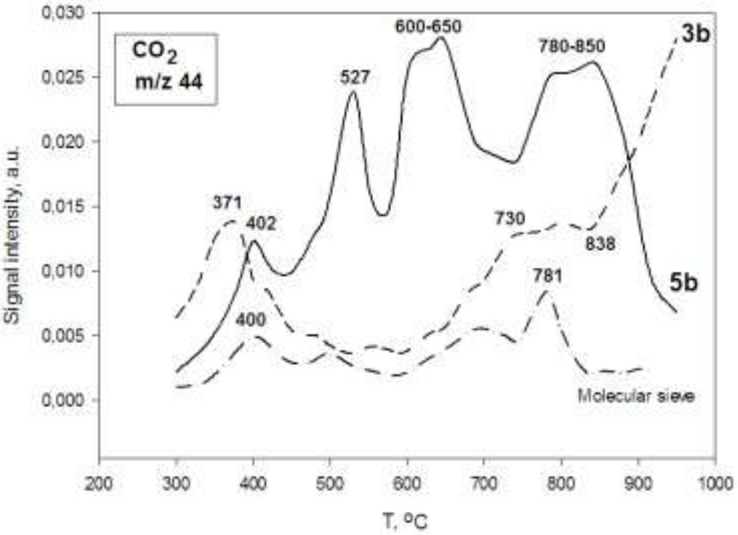

Fig. Thermograms showing dynamics of CO_2 (*m/z* 44) release from the samples CHA (*3b*), HA (*5b*) and «molecular sieve» under heating in vacuum (MX-7304A, SELMI)

Experimentally proved, that physical-chemical parameters of apatites influences on the form of thermograms.

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Influence of nano-additives on hydrogenation properties of R-Mg-Ni-based composites

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Nowadays hydrogen as well as hydrogen containing materials are one of the important sources of alternative energy. Metal hydrides are used for hydrogen storage as well as for negative electrodes of rechargeable Ni-MH batteries. Recently RE-Mg-Ni alloys were developed as promising electrode materials for Ni-MH batteries. R-Ni and RE-Mg-Ni alloys are often studied as composites with Ni (Cu) powders as a binder. In this study we used different types of nanopowders of the Ni, Cu or Ni-based alloys as a binder for the preparation of electrode materials. It was revealed that these nano-additives substantially enhanced the charging-discharging parameters of MH-electrodes. The prepared nano-components as well as the composite materials (R-Mg-Ni alloys with binder nano-additives) were studied in details.

The alloys have been synthesized using arc melting or mechanochemical synthesis, sintering and annealing. Nanopowders of Ni, Cu and alloys were synthesized by the authors and their properties were compared with commercial nano-Ni. The materials were characterized by X-ray diffraction (DRON-3.0 and Bruker-D8 powder diffractometers) and electron probe microanalysis. The gas hydrogenation has been studied using Sivert's type apparatus; electrochemical charge-discharge characteristics were studied using PGStat-8 equipment.

Nanopowders of Ni and Ni-based alloys demonstrated the ability to absorb and desorb hydrogen at ambient conditions. Gas and electrochemical hydrogenation properties of R-Mg-Ni-based composite materials were analyzed to estimate own capacity of the metal hydride components and the capacity of Ni-based nano-additives as hydrogen-sorbing binders. The influence of such additives on properties of composite materials will be discussed in the report. The mechanisms of the observed effects are not clear yet and the possible explanations will be proposed.

Thermodesorption study of surface of bulk Co-Fe catalysts for the reaction of CO_2 hydrogenation

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Carbon dioxide is one of the most used C1 building block in chemical industry as it is a highly functional, abundant, renewable carbon source. The catalytic conversion of CO_2 to methane is a critical goal that should positively impact the global carbon balance by recycling greenhouse gas into usable fuels. Therefore, it is desired to develop an effective catalyst which exhibits both high activity and high resistance to carbonaceous deposit in methanation of carbon dioxide. Non-noble metal-based catalysts are obviously more desirable.

Catalysts were prepared by dissolution of metal in nitric acid with the following precipitation by aqueous ammonia, subsequent drying and reducing the obtained oxides. Experiments were carried out in a fixed-bed system at atmospheric pressure, GSV=100 cm^3 min^{-1} (50% Ar, 48% H_2, 2% CO_2). The surface layer investigations were done by thermally programmed desorption (TPD) with a mass spectrometric detector (MX7304A, Ukraine) of desorbed particles.

A trend of increasing activity with the increasing of Co concentration was observed. The highest yield of methane (100% at 300°C) was obtained on catalyst with 93 wt. % of Co.

TPD MS investigations of the surface layer of this catalyst showed the presence of fragments with *m/z* 18, 28, 44. These signals correspond to H_2O^*, CO^*, CO_2^* particles, relatively. Desorption peaks of these particles have a smooth and symmetrical forms. It is likely that these compounds are dissociated upon adsorption and desorb with second-order kinetics. It is reasonable to assume that, the reaction proceeds according to mechanism that proposes the dissociation of CO_2 with further reduction of carbon species to methane.

Morphology of the obtained catalyst was observed by using scanning electron microscopy (SEM). Synthesized metal particles are highly dispersed, with a size *ca.* 30 nm, agglomerated to 1-100 μm. The surfaces of the agglomerates have a foamy structure, shown a lot of cracks and pores formed by the escaping gases during reduction of the sample.

These results provide some information about mechanism of the methanation. Thus the additional experiments must be conducted in order to discriminate possible mechanisms of the reaction.

Antioxidant properties of exo-derivatives fullerene

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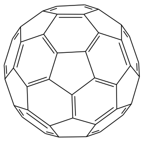
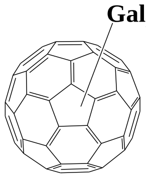
We have obtained results according to the antioxidant exohedral fullerenes properties of the temperature, benzyl alcohol concentration, functionalization degree and functional groups nature in the carbon skeleton.

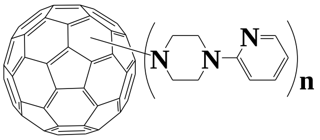
Investigated mechanism of the antioxidative action fullerenes (I)–(XI) under oxidation of model system of benzyl alcohol (40-60 ºC, Po_2 = 0,02–0,1 MPa, initiator – 2,2′-azo-*bis*-isobutyronitril):



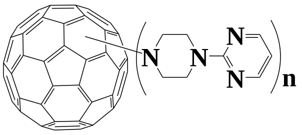
(I),



(II-VI),



(VII-IX),



(X-XI),

where Gal$_n$ = Cl_6, Cl_{12}, Cl_{28}; (VII-IX) – *n* = 6, 8, 14; (X-XI) – *n* = 6, 12.

It is shown that fullerenes break the chains of benzyl alcohol at interaction with alkyl and peroxyl radicals.

Halogenated derivatives of fullerene C_{60} (II-VI) also stoichiometrically inhibit auto- and initiated oxidation of organic substrates. The phenomenon of catalytic termination oxidation chains by exomodified fullerenes with nitrogen-containing heterocyclic substituents (VII-XI) in the model reaction of initiated oxidation of benzyl alcohol was revealed. Nonmonotonic benzyl alcohol (BA) antioxidant properties variation under the chlorine-containing fullerenes action, depending on their chlorination degree, BA concentration (Fig.) and temperature.

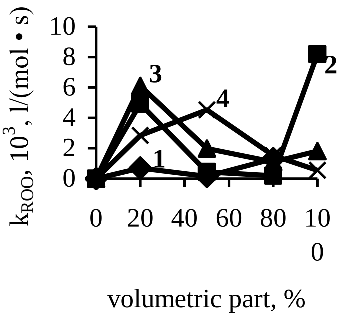


Fig. Dependence of the rate of oxidation chains breaking ($k_{ROO\cdot}$) BA with different concentrations of fullerenes BA in chlorobenzene: *1*- C_{60}, *2*- $C_{60}Cl_6$, *3*- $C_{60}Cl_{12}$, *4*- $C_{60}Cl_{28}$

The correlation analysis of rate constants series of BA oxidation inhibition by chlorine-substituted fullerenes was done. Constants ρ were calculated by Gamete equation for the inhibition rate $k_{ROO}\cdot$and k_R. In case of alkyl radical inhibition were found a high correlation (r >0.99, $\rho_{\text{м}} = 0.026 \pm 0.01$, $\rho_{\text{п}} = 0.043 \pm 0.02$).

The obtained results allow to assess the potential electron opportunities of these compounds for further their using as antioxidants.

Silver nanoparticles in composite systems

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The development of new composites and multi-functional materials based on silver nanophase has received growing interest because of their unique surface effects and many important applications in industry [1-3]. There are attempts to create new composites using silver nanoparticles by involving various types of organic and inorganic solid matrices. For composites based on metal nanoparticles it is necessary to ensure their homogeneous dispersion over the matrix without the formation of large aggregates which could adversely affect the final properties of the materials as well as maintain the narrow size distribution of the nanoparticles [4, 5]. In this work the idea of creating the silver based nanocomposites using low porous colloidal silica materials as synthetic inorganic matrix and chitosan nanofibers as natural polymer matrix is presented. The obtained composites were characterized to illustrate changes of their properties depending on the type of matrix and the synthesis conditions. Particular emphasis has been placed on the distribution of nanosized silver phase on solids and size of silver crystallites, and evaluation of the possible interaction effects between components. Our observations at this stage of work suggest that the choice of the type of silver precursor affords very small crystallites and the mechanism of their reduction (different depending on the matrix type) clearly differentiates the distribution of nanoparticles on the surface. The phenomenon of auto reduction and specific morphology of chitosan nanofibres shows some advantages in comparison to a simple mixture of the constituent elements and the use of thermal reduction (as in the case of using silica support). The role of matrix formed by macromolecular chains of the biocompatible polymer involves improvement of nanoparticles distribution within the material and prevents the aggregates formation. At the same time they play an important role in obtaining a narrow size distribution of the metallic nanoparticles.

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Small-angle X-ray scattering (SAXS) of porous composites

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Desirable features of materials in many applications are connected with developed textural properties like high surface area and high pore volume. The unique properties remain function of nature of the material, the porosity, structure and geometry of pores. Due to the exceptional properties they are object of interest and a real challenge in catalysis, adsorption methods, and many other areas of modern chemistry. Porous silica materials are willingly used as adsorbents, catalyst supports and drug delivery systems due to their high thermal stability, tunable properties, possibility of modification and inactive behaviour in relation to active phases and solvents. Small-angle X-ray scattering (SAXS) measurements based on the elastically scattered X-rays are important in analysis of condensed matter. This procedure allows to obtain the most useful parameters for mesoporous and microporous materials characterization and to compare them successfully with other experimental measurements (for example with experimental nitrogen adsorption/desorption measurements), reducing the time and material consumption with good precision for particles and pores with size below 10 nm. Mesoporous ordered silica nanostructures show strong interaction with X-ray radiation in the range of small-angles. Small-angle X-ray scattering (SAXS) measurements of mesoporous silica materials provides information on the distribution of electron density in the mesoporous material, and allow to determine structure and size of the unit cell as well as type of ordered structure. SAXS can be used to characterize the nanoscale structure both of ordered materials (analysis of position of diffraction peaks) as well as discorded materials. In presented work, the SAXS investigation of structures of a group of porous materials was performed. The properties of mesoporous ordered silica samples as well as active carbon based nanocomposites were evaluated using SAXS technique. The aim of presented work was verification of the procedure of determination of porous structure parameters by SAXS method for mesoporous materials as well as description of the changes of structural properties illustrated by diffraction technique.

Silver nanoparticle formation in micelles and micelle-like structures of heteropolymers

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The noble metal nanoparticles distributed in polymeric matrices are of significant interest due to special optical, electrical, absorption, catalytic, and biocide properties that allows considering them as the advanced materials of modern nanotechnologies. The formation of nanoparticles with necessary size and shape and also the nanoparticle stabilization against aggregation in polymer/metal composites or solutions are the main important problems for their successful application. The method of nanoparticle producing in organic medium due to a metal ion reduction in the reverse micelles of block and graft copolymers is well known. But synthesis of metal nanoparticles in aqueous solutions in hydrophilic polymeric matrices is the most perspective and less toxic from the point of view their biomedical application.

In the present paper, the processes of *in situ* formation of silver nanoparticles (AgNPs) in aqueous solutions of some micelle-forming block and graft copolymers and polymer/inorganic hybrids containing the following chemically complementary components: (methoxy)poly(ethylene oxide)/ polyacrylamide, poly(vinyl alcohol)/polyacrylamide, and silica/polyacrylamide, were compared. The results of studying the effects of chemical nature, molecular architecture and concentration of polymeric matrices and also the content of initial silver salt on the reaction kinetics, size, morphology, yield and stability of AgNPs in aqueous solutions are represented and discussed. They were obtained by ^{1}H NMR and UV-Vis spectroscopy, WAXS, SAXS and TEM methods. The micelles and micelle-like structures of the block and graft copolymers and polymer/inorganic hybrids turned out to be effective nanoreactors, which were capable of ensuring a high rate and efficacy of chemical reduction of Ag+-ions up to nanoparticles with the 2-5 nm size and narrow size distribution. The composites of AgNPs with polymeric and polymer/inorganic matrices showed the two-level fractal organization of their structure. Crystalline AgNPs with a smooth surface were elements of the 1-st lower structural level but the mass-fractal clusters of the matrices constituted the 2-nd higher structural level.

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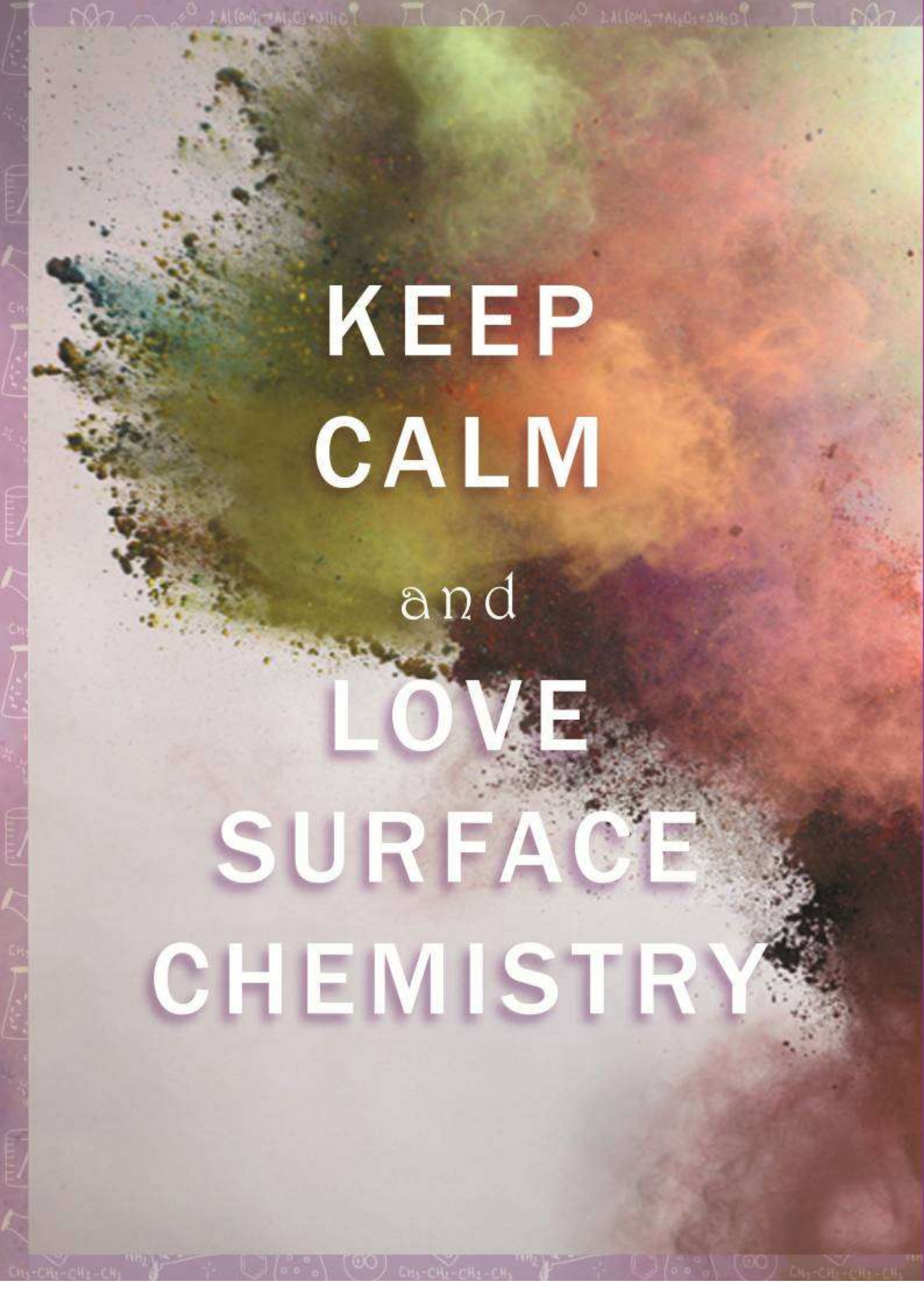
KEEP
CALM
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