

MODERN PHYSICAL CHEMISTRY for ADVANCED MATERIALS

Kharkiv, Ukraine 26 - 30 June, 2014

V.N. Karazin Kharkiv National University, 4 Svoboda Square, Kharkiv, Ukraine

SCIENTIFIC PROGRAM

TYPES OF PRESENTATIONS

Plenary lectures

Keynote and oral symposia presentations

Poster presentations

SYMPOSIA (keynote, oral and poster presentations)

M. New Materials

O. Organized solutions. Green Chemistry

S Solution Chemistry and Electrochemistry

T. Theoretical Chemistry

June 26, 2014 (Thursday)

12⁰⁰: Opening ceremony (Assembly Hall, 2nd floor)

13⁰⁰–14⁰⁰: Lunch ("Bunker" café, Ground floor)

14⁰⁰-18³⁰: **PLENARY LECTURES** (K. Sinelnikov Auditorium, 7th floor)

CHAIRMAN: Alain Walcarius

1. Christian **AMATORE** (France): 'Revisiting the mechanism of vesicular exocytosis based on quantitative treatment of amperometric measurements at ultramicroelectrodes'.
2. Anatoly **POPOV**, Yevgeniy **KARPICHEV** (Ukraine): 'Designing functional microheterogeneous surfactant systems.'
3. Isabelle **RICO-LATTES** (France): 'New "green" trends in galenic: ecodesign of amphiphilic compounds derivated from sugars'.

Coffee-break (30 minutes)

CHAIRMAN: Alexander Korobov

4. Oleg **PREZHDO** (USA): 'Excited state dynamics in nanoscale materials for solar energy harvesting'.
5. Vitaliy **KALCHENKO** (Ukraine): 'Calixarene based supramolecular processes and materials'.
6. Masashi **HOJO**, Yuki **UJI-YIE**, Shohei **TSUBOTA**, Mika **TAMURA**, Akihiko **YAMAMOTO** (Japan): Can pure gold be dissolved in seawater mixed with aqueous nitric acid?

19⁰⁰: Get-together party ("Bunker" café, Ground floor)

June 27, 2014 (Friday) morning

9⁰⁰–12⁵⁰: PLENARY LECTURES (K. Sinelnikov Auditorium, 7th floor)

CHAIRPERSON: **Isabelle Rico-Lattes**

1. Gerbert **KAMALOV** (Ukraine): 'Composition and structure of 3d metals carboxylates and related systems as the activation factors of the hydroperoxides formation and transformation.'
2. Alain **WALCARIUS** (France): 'Electrogeneration of advanced sol-gel materials'
3. Natalya **VODOLAZKAYA** (Ukraine) Solvatochromic indicators as a tool for the investigations of various organized solutions'

Coffee-break (20 minutes)

4. Wolfram **SCHROER** 'Criticality of ionic solutions, ionic liquids and liquid metals'.
5. Yuriy **KHOLIN** 'Physico-chemical characteristics of a medium in the near-surface layer of hybrid silica-organic materials and their influence on adsorption equilibria'.
6. Nikolay **MCHEDLOV-PETROSSYAN** 'Xanthene compounds: unique tools for examining liquid media'.

13⁰⁰–14⁰⁰: Lunch ("Bunker" café, Ground floor)

Afternoon

14⁰⁰–17⁰⁰: PLENARY LECTURES (K. Sinelnikov Auditorium, 7th floor)

CHAIRMAN: **Sergey Shtykov**

7. Armand **LATTES** (France): 'Molecular aggregation in polar non aqueous solvents: interfacial behaviour, micellization, and applications'
8. Alexander **ISHCHENKO**, Andrii **KULINICH** (Ukraine): Merocyanines as functional dyes: Electronic structure, solvatochromism, and application

Coffee-break (20 minutes)

15³⁰–17³⁰: KEY-NOTE LECTURES

CHAIRMAN: **Vitaliy Kalchenko**

9. Edilson **BENVENUTTI** (Brazil): 'Ionic silsesquioxanes: an inexhaustible source of new advanced hybrid materials'.
10. Sergei **SHTYKOV**, Valery **KARTSEV** (Russia): Structural dilatometry of low energy liquid molecular assemblies.
11. Andrey **LYASHCHENKO** (Russia): 'Structure and dynamics of water in electrolyte solutions and its dielectric and thermodynamic properties'.
12. Stepan **KUCHMIY**, Olexandr **STROYUK**, O.E. **RAYEVSKA**, V.M. **DZHAGAN**, M.Ya. **VALAKH** (Ukraine): 'Extremely small metal-chalcogenide nanocrystals: synthesis, photonics, and applications'.

June 28, 2014 (Saturday)

9⁰⁰–11⁵⁰: KEY-NOTE LECTURES (K. Sinelnikov Auditorium, 7th floor) **morning**
CHAIRMAN: **Oleg Prezhdo**

13. Aleksandr **KOROBov** (Ukraine): 'Kolmogorov-Johnson-Mehl Avrami approach in heterogenous chemical kinetics'.
14. Roberto **RIVELINO** (Brazil): 'Structure, thermodynamics and electronic properties of carbon nanostructures via atomistic simulations'.
15. Vladislav **CHERANOVSKII**, Elena **EZERSKAYA**, V. **TOKAREV** (Ukraine): 'Low-temperature thermodynamics of one-dimensional models for transition metal polymeric compounds'.

Coffee-break (20 minutes)

1. Oleg **KALUGIN**, B.A. Marekha, A.V. Riabchunova, A.K. Adya, I.V. Voroshylova, O.V. Lukinova, V.V. Chaban, A. Idrissi (Ukraine): 'Structure and Dynamics of Room Temperature Ionic Liquids and their Mixtures with Molecular Liquids'.
2. Dmitriy **NERUKH**, Arturs Scukins, Evgen Pavlov, Sergey Karabasov, Anton Markesteijn (Great Britain): 'Hybrid molecular dynamics–hydrodynamics framework for modelling liquid molecular systems'

12⁰⁰–13⁰⁰ POSTER SECTION (foyer of the Assembly Hall, 2nd floor)

13⁰⁰–14⁰⁰: Lunch ("Bunker" café, Ground floor)

14⁰⁰–16⁴⁵ SYMPOSIA (with 20 minutes coffee-breaks):

O. Organized solutions. Green Chemistry (Conference hall, Auditorium 2-49, 2nd floor)

M. New Materials (K. Sinelnikov Auditorium, 7th floor)

17⁰⁰–18⁰⁰: POSTER SECTION (foyer of the Assembly Hall, 2nd floor)

June 29, 2014 (Sunday)

9⁰⁰–11⁴⁵: SYMPOSIA (with 20 minutes coffee-breaks):

S. Solution Chemistry (N. Komar Auditorium 7-79, 7th floor)

T. Theoretical Chemistry (K. Sinelnikov Auditorium, 7th floor)

12⁰⁰–13⁰⁰ POSTER SECTION (foyer of the Assembly Hall, 2nd floor)

13⁰⁰–14⁰⁰: Lunch ("Bunker" café, Ground floor)

14⁰⁰–16⁴⁵: SYMPOSIA (with 20 minutes coffee-breaks):

S. Solution Chemistry (N. Komar Auditorium 7-79, 7th floor)

T. Theoretical Chemistry (K. Sinelnikov Auditorium, 7th floor)

17⁰⁰-18⁰⁰: POSTER SECTION (foyer of the Assembly Hall, 2nd floor)

June 30, 2014 (Monday)

9⁰⁰-11⁴⁵: SYMPOSIA (with 20 minutes coffee-break):

O. Organized solutions. Green Chemistry (Conference hall, Auditorium 2-49, 2nd floor)

S. Solution Chemistry (N. Komar Auditorium 7-79, 7th floor)

T. Theoretical Chemistry (K. Sinelnikov Auditorium, 7th floor)

12⁰⁰-13⁰⁰: POSTER SECTION (foyer of the Assembly Hall, 2nd floor)

13⁰⁰-14⁰⁰: Lunch ("Bunker" café, Ground floor)

Afternoon: social program

SYMPOSIA

O. Organized Solutions. Green Chemistry (June 28, 2014) afternoon

CHAIRPERSONS: **Lucia Zakharova, Sergey Shtykov, Nataliya Vodolazkaya**

ORAL PRESENTATIONS			
1	<u>Zakharova L.Ya.</u>	Russia	Supramolecular systems based on amphiphiles and polymers: design, self-organization and guest-host interactions
2	<u>Kulikov A.Yu.,</u> Renkevich A. Yu.	Ukraine	Giddings model for micellar and submicellar thin layer chromatography
3	<u>Kapitanov I.V.,</u> Belousova I.A., Shumeiko A.E., Kostrikin M.L., Prokop'eva T.M., Karpichev E.A., Popov A.F.	Ukraine	Micellar effects of oximate-functionalized monomeric and gemini surfactants in acyl groups transfer
4	<u>Fomina E. S.,</u> Vysotsky Yu.B.	Ukraine	Quantum-chemical assessment of clusterization thermodynamics of N-acylsubstituted alanine at the air/water interface
5	<u>Bykov A.G.,</u> Lin S.-Y., Noskov B.A	Russia	Surface dilational viscoelasticity of polyacid/dodecyltrimethyl ammonium bromide solutions
6	<u>Kyrychenko A. V.,</u> Korsun O. M., Gubin I. I., Kovalenko S. M. and Kalugin O. N.	Ukraine	Molecular dynamics simulations of silver nanoparticles coated with poly-vinylpyrrolidone
7	<u>Milyaeva O.Yu.,</u> Noskov B.A., Lin S.-Y., Loglio G., Miller R.	Russia	Dynamic surface properties of mixed protein-polyelectrolyte solutions.
8	<u>Y. Açıkbaş,</u> R. Çapan, M. Erdoğan and F. Yukruk	Turkey	An investigation of 1,7- dibromo- N,N'-(bicyclohexyl)-3,4:9,10- perylendiimide Langmuir-Blodgett film for organic vapor sensing using surface plasmon resonance technique

M. Material Science (June 28, 2014) afternoon

CHAIRMAN: **Aleksandr Korobov**

ORAL PRESENTATIONS			
1	<u>Pud A.A.</u> , Ogurtsov N.A., Noskov Yu.V., Fatyeyeva K.Yu., Ilyin V.G.	Ukraine	Role of physical-chemical interactions in structure-property relationship of the conducting polymer shells at template cores
2	<u>Lobko Eu.V.</u> , Meshkova S.B., Topilova Z. M., Kyriak A.O, Doga P.G., Klepko V.V.	Ukraine	Photo stability of europium complex in polyurethane matrixes of different structure and topology
3	<u>Gautam Surendra K.</u>	Nepal	XRD and TEM: characterizing tools for analysing group II-VI semiconductor nanoparticles
4	<u>Adiguzel O</u>	Turkey	Phase transitions and nanoscale design of martensite in copper based shape memory aloys
5	<u>Lutsyk V.I.</u> , Vorob'eva V.P., Shodorova S.Ya.	Russia	T-x-y diagrams space models for the lead-free solders
6	<u>Lukyanov Boris</u> , Tyurin Roman, Chernyshev Anatoliy, Lukyanova Maria, Mukhanov Evgeniy, Ozhogin Ilya, Komissarova Oksana , Doroshenko Andrey, Roshal Alexander	Russia	New Spirocyclic System Design for Light Operated Elements for Molecular Photonics

T. Theoretical Chemistry (June 29, 2014) morning

CHAIRPESONS: **Vladislav Cheranovskii, Vladimir Ivanov**

ORAL PRESENTATIONS			
1	<u>Doroshenko A.O.</u>	Ukraine	Intramolecular excited state proton transfer reaction and H-bonding impurities: theoretical modeling
2	Shahriar Ghammamy, <u>Elahe Yousefy</u>	Iran	Density functional theory studie of structural properties , Natural Bond Orbital, and Energies for the 1,3–benzoxazine derivatives
3	<u>Qaitmas Noorahmad,</u> Ghammamy Shahriar	Iran	Structural Properties, Natural Bond Orbital, Theory
4	<u>Ahmadzadeh Farnaz,</u> Ghammamy Shahriar	Iran	Density functional theory study the 2-(2,4-difluorophenyl)-4,5-dimethyl-1- (4-methylphenyl)-1h-imidazole

S. Solution Chemistry and Electrochemistry (June 29, 2014) morning

CHAIRPESONS: **Alexander Dikusar, Oleg Kalugin**

ORAL PRESENTATIONS			
1	<u>Dikusar A.I.</u>	Moldova Republic	Induced codeposition of CoW coatings from citrate and gluconate solutions. Role of complexation
2	<u>Al-Kahali Mohamed S. N.,</u> Abduljabbar Adlia A. M.	Yemen	Aquatic Photo-Catalytic Degradation of Textile Dyes and Pesticides Using Different Catalysts Under UV-Lamp Radiation And Sunlight (At Altitude of 2700 m Above Sea-Level)
3	<u>Shahbazkhany Saeedeh,</u> Ghammamy Shahriar	Iran	Structural properties, natural bond orbital, Density Functional Theory Calculations For 2-[(1H-Pyrrol-2-yl)methyl]-1H-pyrrole
4	<u>Sokolova I.V.,</u> Vershinin N.O., Tchaikovskaya O.N., Nevolina K.A.	Russia	The direct and sensitized photolysis of organochlorine compounds under exilamps irradiation in water solutions
5	<u>Oleinick A.,</u> Zhu F., Yan J., Mao B., Svir I., Amatore C.	France	Theoretical investigation of generator-collector microwell arrays for improving electroanalytical selectivity. Application to selective dopamine detection in presence of ascorbic acid.

6	Philippe P. Lainé, Jérôme Fortage, Grégory Dupeyre, Christian Perruchot, Fabien Tuyères, Magdaléna Hromadová, Lubomir Pospíšil, Štěpánka Lachmanová, Ján Tarábek, Sophie Griveau, Fethi Bedioui, Cyril Peltier, Ilaria Ciofini and Carlo Adamo	France	The pyridiniums revisited: further expanding their electrochemical versatility with a new electrochemical paradigm
7	Roshal A.D., Serdiuk I.E., Varenikov A.S.	Ukraine	7-Hydroxyflavone Revisited: Spectral, Acid-Base Properties and Interplay of Protolytic Forms

O. Organized Solutions. Green Chemistry (June 30, 2014) morning

CHAIRPERSONS: Lucia Zakharova, Sergey Shtykov, Nataliya Vodolazkaya

ORAL PRESENTATIONS			
1	Glebov E.M., Semionova V.V., Korolev V.V., Sapchenko S.A., Samsonenko D.G., Fedin V.P., Shirinian V.Z.	Russia	Supramolecular adducts formed by organic photochroms and the metal-organic coordination polymer
2	Mikhaylov S., Pud A., Wojkiewicz J-L., Redon N.	France	Synthesis and investigation of conducting polymer based nanocomposites for ammonia detection
3	Aydemir Tülin, Güler Semra, Becerik Seda Çınar, Eser Ahmet, Dinçer Ayşe	Turkey	The preparation of histidine modified chitosan beads for enzyme immobilization
4	Anishchenko V.N., Rybachenko V.I., Chotiy K. Yu., Redko A.N.	Ukraine	Application of inverse phase transfer catalysis in organic chemistry
6	Telbiz G.M., Leonenko E.V., Bogoslovskaja A.B., Manorik P.A.	Ukraine	The effect of mesoscopic ordering of dye molecules on the optical properties of composite sol-gel coating
7	Kalchenko O.I., Drapailo A.B., Shishkina S.V. , Shishkin O.V. , Kharchenko S.G., Gorbachuk V.V., Kalchenko V.I.	Ukraine	Complexation of thiacalix[4]arene methylphosphonic
8	Czechowska-Kryszk J., Holec-Gąsior L., Ferra B., Serdiuk I., Krzywiński K.	Poland	Performance of new acridinium luminescent labels employed in simple immunodiagnostic tests

S. Solution Chemistry and Electrochemistry (June 30, 2014) morning

CHAIRPESONS: **Alexander Dikumar, Oleg Kalugin**

ORAL PRESENTATIONS			
1	<u>Agieienko V.N.</u> , Smortsova Ye.Yu., Kolesnik Ya.V., Kalugin O.N.	Ukraine	Ion association and solvation of double charged metal perchlorates in acetonitrile media: a joint molecular dynamics and electrical conductivity investigation
2	<u>Riabchunova A.V.</u> , Gavriukova Ie.O., Kalugin O.N.	Ukraine	Self-association of room temperature ionic liquids in diluted solutions: aqua medium against non-aqueous solvents
3	<u>Malek Naved I</u>	India	Interaction between Ionic Liquids and Gemini Surfactant: A Detailed Investigation into the Role of Ionic Liquids in Modifying Properties of Aqueous Gemini Surfactant
4	<u>Samarov A.A.</u> , Toikka M.A., N.S.Tsvetov, Toikka A.M.	Russia	Experimental study of solubility and liquid-liquid equilibria in quaternary system acetic acid – n-propanol – n-propyl acetate – water
5	<u>Rajni Mathur</u> and Meeta Trivedi	India	Electrosynthesis of epoxy resins via superoxide anion
6	<u>Suleimenov I.E.</u> , Utelbayev B.T., Myrzakhanov M.M., Suleimenov E.N.	Republic of Kazakhstan	Mechanism of Electrophoretic Mobility of Micro- and Macro-Inclusions in Liquid Systems

T. Theoretical Chemistry (June 30, 2014) morning

CHAIRPESONS: **Vladislav Cheranovskii, Vladimir Ivanov**

ORAL PRESENTATIONS			
1	<u>Latelli Nadjia</u> , Ouddai Nadia, Arotçaréna Michel, Chaumont Philippe, Mignon Pierre and Chermette Henry	Algeria	Mechanism of addition-fragmentation reaction of thiocarbonyls compounds in free radical polymerization. A DFT study
2	<u>Hedayaty Roya</u> , Ghammamy Shahriar	Iran	The Nitrophenyl-1,2,3-Triazole roles as anti-HIV and anti-Cancer:a theoretical investigation
3	<u>Babahedari Ali Kazemi</u> , Faraji Somayeh, Soureshjani Ehsan Heidar	Iran	A Comparative Molecular Docking study of Lavandula Angustifolia Mill's compounds With GABAA Receptor
4	<u>Laktarashy Fatemeh</u> , Ghammamy Shahriar	Iran	theory functional calculations ,Natural Bond Orbital and Structural Properties of 2-sulfanyl-

			ideneimidazolidin-4-one
5	Haghnejad Samira , Ghammamy Shahriar	Iran	Structural Properties, Natural Bond Orbital, Density Functional Theory (DFT), and theoretical study for the Ethyl (2E)-2-cyano-3-(4-methoxyphenyl)- acrylate and derivatives with fluorine
6	Bagheri Maedeh, Ghammamy Shahriar	Iran	Theoretical investigation of natural bond orbital, density functional theory and structural properties of anthracene tetraone

POSTER PRESENTATIONS
June 28-30, 2014

O. Organized Solutions. Green Chemistry

1.	<u>Chernysheva O.S.</u> , Reshetnyak E.A., Mchedlov-Petrossyan N.O.	Ukraine	The study of premicellar aggregation of the sodium salts of alkyl sulfonate	
2.	Karpichev Ye.A., <u>Chernyshova V.V.</u> , Zubareva T.M., Prokop'eva T.M.	Ukraine	Micellar effects of cationic gemini surfactants on the nucleophilicity of hydroxide ion and alpha nucleophiles	
3.	<u>Fihurka N.V.</u> , Varvarenko S.M., Dron I.A., Ferens M.V., Vostres V.B.	Ukraine	Surface active properties of pseudo-poly(amino acid)s of a polyester type	
4.	<u>Govor I.V.</u> , Tatarets A.L., Dyubko Tatyana, Terpetschnig E.A., Patsenker L.D.	Ukraine	Effect of urea on the interaction of the fluorescent squaraine dyes Square-634 and Square-685 with serum albumin	
5.	<u>Govor I.V.</u> , Tatarets A.L., Obukhova O.M., Terpetschnig E.A., Patsenker L.D.	Ukraine	Förster resonance energy transfer (FRET) between environment-sensitive squaraine dyes to detect the conformational changes in proteins	
6.	<u>Hubina A.V.</u> , Lobko Ye. V., Fomenko A.O.	Ukraine	Structure peculiarities of polymer films based on xanthan and citric acid	
7.	<u>Kamneva N.N.</u> , Mchedlov-Petrossyan N.O.	Ukraine	Protolytic equilibrium of indicator dyes in cationic surfactant-based reversed microemulsions	
8.	<u>Kharchenko A.Yu.</u> , Kamneva N.N., Mchedlov-Petrossyan N.O.	Ukraine	Protolytic equilibrium of indicator dyes in cationic surfactant-based solutions with adding of butanol-1	
9.	<u>Pushkarevskaya E.V.</u> , Vodolazkaya N.A.	Ukraine	Spectroscopic study of acid-base ionization and tautomerism of fluorescein dyes in micellar solutions of cationic dimeric surfactant	
10.	<u>Krasnopyorova A.P.</u> , Efimova N.V., Borisovskaya V.A.	Ukraine	The sorption of radionuclides ⁹⁰ Sr and ¹³⁷ Cs by modified natural biopolymer	
11.	<u>Laguta A. N.</u> , Eltsov S. V.	Ukraine	Micellar and salt effects in kinetics of interaction of phenolphthalein with hydroxide ion	
12.	<i>Mokhtari</i>	<i>Algeria</i>	<i>The influence of boric acid, on the electrochemical behaviour and on the electrodeposits morphology for Co on Platinum substrate.</i>	?

13.	<u>Posokhov Y.O.</u> , Pasiuga V.N., Shckorbatov Y.G.	Ukraine	Derivatives of 2,5-diaryl-1,3-oxazole as fluorescent probes to monitor the changes in human erythrocyte membranes under the influence of magnetic field or electromagnetic radiation
14.	<u>Shvets O.M.</u> , Lyashenko D.Yu., Belyakova L.A.	Ukraine	Study of cadmium (II) trace amounts sorption by β -cyclodextrin-containing silicas in the presence of salts of water hardness
15.	<u>Singh Namrata</u> , Karpichev Yevgen, Ghosh Kallol K.	India	Reactivity of charged and uncharged oximes against decontamination reactions in cationic micellar aggregates: relevance to gemini surfactants
16.	<u>Sursyakova V.V.</u> , Burmakina G.V., Rubaylo A.I.	Russian Federation	Investigation of supramolecular associates between metal complexes and β -cyclodextrin using capillary electrophoresis
17.	<u>Yukhno G.D.</u> , Krasnopyorova A.P., Archipov O.A.	Ukraine	Thermodynamics extraction of zinc in water system with two phases: polyethylene – magnesium sulphate – water
18.	Vasilieva E.A., Lukashenko C. C., Ibragimova A.R., <u>Zakharova L.Ya.</u>	Russia	The polymer-colloid complexes based on gemini surfactants and polyacrylic acid. The role of structural factor
19.	<u>Zhiltsova E.P.</u> , Pashirova T.N., Lukashenko S.S., Valeeva F.G., Gaysin N.K., Gnezdilov O.I., Zakharova L.Ya., Konovalov A.I.	Russia	1. Supramolecular catalytic systems based on quaternary 1,4-diazabicyclo[2.2.2]octane and lanthanum nitrate. 2. Self-organization of the novel amphiphiles bearing three pyrimidine fragments
20.	<u>Kryklya S.O.</u> , Malysheva M.L., Samchenko Yu.M.	Ukraine	Hybrid hydrogels with enhanced properties
21.	<u>Roshchina E.V.</u> , Eltsov S.V., Mchedlov-Petrossyan N.O.	Ukraine	Micellar rate effects in the reactions of alkaline fading of some triphenylmethane dyes
22.	<u>Sliusar Yu.S.</u> , Samchenko Yu.M., Malysheva M.L.	Ukraine	Thermosensitive nanosized hydrogels based on N-isopropylacrylamide for design of targeted drug delivery systems
23.	Siddiq Mohammad and Ambreen Jaweria	Pakistan	Effect of topology of poly(acrylic acid) on cloud point temperature of poly(2-ethyl-2-oxazoline).
24.	<u>Natalia A. Leonova</u> , <u>Anatoliy V. Drozd</u>	Ukraine	The determination of concentrations of Ni^{2+} , Co^{3+} , Fe^{2+} , Cu^{2+} with 1-(2-pyridylazo)-2-naphthol in aqueous-micellar medium on two-intensive parameters
25.	<u>Ryazanova O.A.</u> , Voloshin I.M., Glamazda A.Yu., Karachevtsev V.A., Ilchenko M.M., Dubey I.Ya., Zozulya V.N.	Ukraine	The features of polyphosphate-induced aggregation of multicharged cationic meso-porphyrins: spectroscopic study

T. Theoretical Chemistry

1.	<i>Ahmady</i>	<i>Iran</i>	<i>Theory functional calculations, natural bond orbital, dipole moment and energies for organofluorines chemistry compounds</i>	?
2.	<u>Berdnik M. I.</u> Zakharov A. B. Ivanov V. V.	Ukraine	Coulson–Longuet–Higgins atom-atomic polarizabilities as electronic conductivity parameter of carbon nanotubes	
3.	Masalitina N.Yu., <u>Bliznjuk O.N.</u> , Ogurtsov A.N.	Ukraine	Low-temperature thermodynamics of defect inactivation in rare-gas solids	
4.	<u>Dyakonenko V.V.</u> , Shishkin O.V.	Ukraine	Role of electrostatic interactions in the formation of supramolecular architecture of molecular crystals: case of caged heterocycles	
5.	<i>Ghammamy</i>	<i>Iran</i>	<i>Structural properties , natural bond orbital , Density Functional Theory Calculations For</i>	?
6.	<u>Streltsova E.A.</u> , Grosul A.A., Popova I.V.	Ukraine	Adsorption of Tweens and dodecylpyridinium chloride from binary water solutions on paraffin	
7.	<u>Halauko Y.S.</u>	Belarus	DFT calculated equilibrium CH acidity of nitrogen-containing heterocycles: a hint for regioselective functionalization	
8.	<u>Hannachi D.</u> , Ouddai N.	Algeria	The computational investigations on addition-fragmentation reaction of thioesters compounds in free-radical polymerization	
9.	<u>Karimi Tahereh</u> Ghammamy Shahriar	Iran	Natural bond orbital ,theory functional calculations (DFT), structural properties, and energies for (3ar,6S,7ar)-7a-Chloro-6-methyl-2-(4 nitro phenyl sulfonyl) -1,2,3,6,7,7a-hexahydro-3a,6-epoxyisoindole	
10.	<i>Kravchenko</i>	<i>Ukraine</i>	<i>On the energy spectrum of t-J model on the distorted «necklace ladder »</i>	?
11.	Marekha B.A., <u>Filatov Ya.I.</u> , Kalugin O.N., Idrissi A.	Ukraine, France	Multiple non-covalent interactions in the ion pairs of 1,3-dialkylimidazolium ionic liquids	
12.	<u>Medviediev Volodymyr V.</u> , Shishkin Oleg V.	Ukraine	Relationship between supramolecular architecture and mechanical properties of crystals of CDNA polymorphs	
13.	Zekri S., <u>Ouddai N.</u>	Algeria	Time dependent density functional study of the absorption spectra of thiocarbonyl compounds used in RAFT polymerisation	
14.	<u>Riazikia Mehrdad</u> , Mohammadi Nahid	Iran	Substitution effect on syn and anti conformations of 2-pyridylcarbene	
15.	<u>Savchenko V.S.</u> , Zimin A.A.	Russian Federation	Geometry optimization and the subsurface states of nanodiamond	
16.	<u>Shishkina S.V.</u> , Berski S., Latajka Z., Shishkin O.V.	Ukraine	Intramolecular interactions within FONO molecule.	

17.	<u>Solomonov A.V.</u> , Serebryakova M.K., Uckhov P.V., Rumyantsev E.V.	Russian Federation	Kinetics and mechanism of bilirubin oxidation reactions in polar solvents
18.	Ulacco S., <u>Simonetti S.</u>	Argentina	Platinum-nickel catalysts: advanced materials for cis-oleic acid adsorption
19.	Timchenko O. V., <u>Sokolova I. V.</u> , Kopylova T.N.	Russia	Effect of substitution on spectral-luminescent properties styryl-substituted benzene derivatives
20.	Ghammam Shahriar <u>Yousefi Farzane</u>	Iran	Structural properties, theory functional calculations (DFT), natural bond orbital and energies for the N-(3-chloro-1H-indazol-5-yl)-4-methoxybenzenesulfonamides
21.	<u>Zakharov A. B.</u> , Ivanov V. V.	Ukraine	New π -electron approach for optical properties calculation in the framework of local coupled cluster theory
22.	<u>Zhikol O.A.</u> , Fokin A.A., Shishkin O.V.	Ukraine	Are substituent steric effects dominantly repulsive?
23.	<u>Vechorkina O.V.</u> , Zaporozhets I.A. Ivanov V.V.	Ukraine	Logistic regression in classification of polycyclic aromatic hydrocarbons
24.	<u>Vovchynskiy I.S.</u> , Kalugin O.N., Prezhdo O.V.	Ukraine	Water influence on electronic properties of single-walled carbon nanotubes
25.	<u>Koverga V.A.</u> , Lipeuko A.S., Voroshylova Iu.V., Kolesnik Ya.V., Idrissi A., Kalugin O.N.	Ukraine	The force field models for the molecular dynamics simulations of room temperature ionic liquids

S. Solution Chemistry and Electrochemistry

1.	<u>Bondarev N.V.</u>	Ukraine	Electrostatic and electrochemical approaches to formation of electrical double layer of cationic surfactants micelles
2.	<u>Bondaryev S.N.</u> , Bondaryev N.V.	France	Neural network modeling of medium properties influence at thermodynamics of acetic acid dissociation in solution
3.	<u>Bulavko G.V.</u> , Davidenko N.A., Studzinsky S.L., Derevyanko N.A., Ishchenko A.A.	Ukraine	Effect of electron-donating ability of heteroresidue on the photovoltaic properties of nanocomposites based on symmetric cation polymethine dyes
4.	<u>Cheipesh T.A.</u> , Mchedlov-Petrosyan N.O., Vodolazkaya N.A., Roshal A.D., Shekhovtsov S.V.	Ukraine	Ascertained new features of tautomerism and fluorescence of fluorescein dyes in solution
5.	<u>Cherginets V.L.</u> , Rebrova T.P., Naumenko V.A.	Ukraine	On oxoacidic properties of some melts based on alkali metal bromides
6.	<u>Cirocka A.</u> , Wcisło A., Nakonieczna S., Niedziałkowski P., Zarzczańska D., Ossowski T.	Poland	Acid-base and complexing properties of anthraquinone derivatives with polyether substituents
7.	Krzywiński K.J., Serdiuk I., <u>Czechowska-Kryszk J.</u>	Poland	Poly-acridinium esters – new and promising luminogenic molecules for ultra-sensitive analytical applications
8.	<u>Efimov P.V.</u> , Kalugin O.N.	Ukraine	The new approach for determination of limiting transference numbers from EMF measurements
9.	<u>Gagolkina Z. O.</u> , Lobko Eu.V., Lysenkov E.A., Yakovlev Yu.V., Klepko V.V.	Ukraine	Conductivity of cross-linked polyurethanes, modified with multiwalled carbon nanotubes
10.	Slepushkin V.V., <u>Gukin A.Ye.</u> , Rublinskaya J.V., Ilinykh E.O.	Russia	Local cyclic voltammetry in kinetic study of oxide layers on metals and alloys during anodic polarization in alkaline solutions
11.	<u>Kheireddine A.</u> , Fahim I., Belaouad S.	Morocco	Beta[Sr(PO ₃) ₂] as a novel corrosion inhibitor for mild steel in 1 M HCl
12.	Kalitevskaya E. N., <u>Krutyakova V. P.</u> , Razumova T. K., Starovoytov A. A.	Russia	The mechanisms of the formation of the component composition for molecular layers and solutions of symmetric polymethine dyes

13.	<u>Krzywiński K.J.</u> , Serdiuk I.	Poland	Poly-acridinium esters – new and promising luminogenic molecules for ultra-sensitive analytical applications	
14.	<u>Kuznetsova</u>	Russian Federation	Local structure characteristics of 3:1 and 1:3 aqueous electrolyte solutions at 25 °C.	?
15.	<u>Lefedova O.V.</u> , Nguyen Thi Thu Ha	Russia	Liquid-phase hydrogenations of nitrobenzene and nitrosobenzen on nickel Raney	
16.	<u>Lyga R.I.</u> , Leonova N.G., Zhil'tsova S.V., Gurtovoj D.V., Mikhal'chuk V.M.	Ukraine	Anticorrosive properties of epoxy-silica coatings of aluminum alloys	
17.	<u>Mayba</u>	Ukraine	Electrodeposited cobalt and irperspective electrochemical energy storage – redox flow batteries	?
18.	<u>Mayba M. V.</u> , Sakhnenko N. D., Ved M. V., Bairachnaya T. N.	Ukraine	Perspective electrochemical energy storage – redox flow batteries	
19.	<u>Merouani</u>	Algeria	DFT study of the synthesis of nitrogenated heterocycles of six and seven links	?
20.	<u>Nakoneczna S.</u> , Zięba P., Cirocka A., Niedziałkowski P., Zarzeckańska D., Ossowski T.	Poland	Spectroscopic and electrochemical investigations into the acid-base properties of mono and di-aza 12-crown-4-ethers substituted by anthraquinone moiety	
21.	<u>Nakoneczna S.</u> , Wcisło A., Wnuk E., Niedziałkowski P., Zarzeckańska D., Ossowski T.	Poland	Electrochemical and spectroscopic properties of aza-crown ethers with anthraquinone moiety integrated into macrocyclic ring	
22.	<u>Ossowski T.</u> , Wcisło A., Zięba P., Wnuk E., Niedziałkowski P., Zarzeckańska D.	Poland	Spectroscopic and electrochemical properties of 1-amino-8-chloroanthraquinone derivatives	
23.	<u>Panteleimonov A.</u> , Tkachenko O., Kholin Yu., Gushikem Y.	Ukraine	A novel electrochemical sensor based on silica modified with 1-methylimidazolium chloride	
24.	<u>Povar Igor</u> , <u>Spinu Oxana</u>	Moldova	Correlation between differential equilibrium expressions and the temperature dependence of stability coefficients in three-component systems	
25.	<u>Pushkarova Ya.N.</u> , <u>Solodovnik O.S.</u> , Panchenko V.G., Kholin Yu.V.	Ukraine	Prediction of the solubility of 1-1 electrolytes in nonaqueous solvents with the use of the radial basis function artificial neural network	

26.	Acar H., Karakisla M., Aksu L., <u>Saçak M.</u>	Turkey	Corrosion protection of electrodeposited conductive poly(o-toluidine) on 316 steel electrode
27.	<u>Sanin E.V.</u> , Novikov A.N., Roshal A.D.	Ukraine	Electronic structure and fluorescent properties of 2-(3-coumaroyl)-benzopyrylium salts
28.	<u>Serdiuk I.E.</u> , Roshal A.D., Błażejowski J.	Ukraine	Derivatives of flavilium cations as potential ESIPT fluorophores
29.	<u>Tomaš R.</u> , Bešter-Rogač M., Jovanović	Croatia	Viscosity <i>B</i> -coefficient for sodium chloride in aqueous binary mixtures of 1,4-dioxane
30.	<u>Tsurko E.N.</u>	Ukraine	Quantitative description of the biomolecule solvation in solutions of two- and three-basic amino acids, their salts and derivatives
31.	<u>Zieba P.</u> , Wnuk E., Cirocka A., Fabianska A., Bogdanowicz R., Ossowski T.	Poland	Boron doped diamond (BDD) electrodes- electrochemical properties and surface modification.
32.	<u>Cherginets V.L.</u> , Rebrova T.P., Naumenko V.A., Ponomarenko T.V.	Ukraine	Features of carbobromination of KBr-NaBr equimolar melt
33.	Mchedlov-Petrosyan N.O., <u>Mahmood Y. T.</u> , Shekhovtsov S. V., Tkachenko E. A., Gromovoy T. Yu.	Ukraine	Coagulation of organosols of fullerene C ₆₀ by electrolytes
34.	<u>Goga S. T.</u> , Lebed A. V., Mchedlov-Petrosyan N. O.	Ukraine	Association and transport properties of symmetrical and asymmetrical tetraalkylammonium perchlorates in non-hydrogen bond donor solvents
35.	<u>Petrenko N.O.</u> , Panchenko V.G., Krasnoperova A.P., Yukhno G.D., Kalugin O.N.	Ukraine	Solubility of lithium bis-(oxalate) borate in ethylacetate
36.	<u>Amatore Ch.</u>	France	Transport and Reactivity in Molecular Electrochemical Mechanisms: Bridging the Gap between Molecular and Electrocatalytic Fields
37.	<u>Babanly D.M.</u> , Sukurova G.M., Aliev A.Sh.	Azerbaijan	The thermodynamic properties of Tl ₅ Te _{3-x} Br _x solid solutions
38.	<u>Ibadova G.I.</u> , Aliev Z.S., Veysova S.M., Babanly M.B.	Azerbaijan	Thermodynamic investigation of solid solutions Yb _x Pb _{1-x} Te by EMF method

39.	Panchenko V.G., Onischenko Lukinova <u>Lyashenko D.A.</u> , Kalugin O.N.	V.K. E.V.,	Ukraine	Electroconductivity and ion association to pairs and triple ions in ethyl acetate solutions of lithium bis-(oxalato)borates
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M. New Materials

1.	<u>Barakov R. Yu.</u> , Shcherban N.D., Yaremov P.S., Solomakha V.M., Ilyin V.G.	Ukraine	Low-temperature synthesis, structural-sorption properties and acidity of micro-mesoporous aluminosilicates obtained from sol-precursor of zeolite ZSM-5	
2.	<u>Bairachnaya T.N.</u> , Ved M.V., Sakhnenko N.D., Glushkova M.A., Karakurkchi A.V.	Ukraine	Electrodeposited cobalt and iron alloys as materials for ecotechnology	
3.	<u>Tahar N. Ben</u> , Mimoun H.	Algeria	Synthesis of catalysts and application in petroleum refining	
4.	<i>BEN TAHAR</i>	<i>Algeria</i>	<i>Preparation of solid catalysts and its application for conversion of heavy petroleum fractions</i>	?
5.	<i>BEN TAHAR</i>	<i>Algeria</i>	<i>Valorization of petroleum loads by thermal process</i>	?
6.	<u>Bulgakova A.V.</u> , Sofronov D.S., Chebanov V.A.	Ukraine	Sorption properties of ZnS towards metals	
7.	<u>Danilov F.I.</u> , Protsenko V.S., Vasil'eva E.A., Amirulloeva N.V., Smenova I.V.	Ukraine	Electrodeposition of Fe and Fe-ZrO ₂ composite coatings from methanesulphonate baths	
8.	<u>Daoui A.</u> , Safi B., Rezak M.	Algeria	Use of waste wood (Aleppo pine) as superplasticizer in an new concrete (self-compacting concrete): effect on rheological and physico-mechanical	
9.	Schneid A. C., Roesch E. W., Sperb F., Matte U., da Silveira N. P., Costa T. M. H., Benvenuti E. V., <u>de Menezes E. W.</u>	Brazil	Silver nanoparticles/ionic silsesquioxane new system: a synergistic effect in antibacterial activity	
10.	Denisov S.I., Lyutyy T.V., <u>Pedchenko B.O.</u> , Babych H.V.	Ukraine	Heating of nanocomposites containing single-domain metal particles	
11.	<u>Fedyunyayeva I.A.</u> , Povrozin Ye.A., Tatarets A.L., Sidorov V.I., Terpetschnig E.A., Patsenker L.D.	Ukraine	Long-wavelength fluorescent dye for lifetime sensing in acidic media	

12.	<u>Honcharov V.</u> , Zazhigalov V., Kowal A., Colombi P.	Ukraine	Structural, catalytic and thermal properties of stainless steel after ionic implantation
13.	<u>Karaush N. N.</u> , Baryshnikov G. V., Minaev B. F.	Ukraine	Design of nanoscaled 1d and 2d materials based on tetraoxa[8]circulene
14.	<u>Klypa K.I.</u> , Veselovskyi V.L., Diyuk V.E., Ischenko E.V.	Ukraine	Functionalization of surface layer of activated carbon by bromination and amination
15.	<u>Kovtun G.I.</u> , Konoplia M.M., Dydiuk M.V., Yashchenko G.V., Mysiura A.G.	Ukraine	Wound dressing based on nonwoven fabrics with multi-layered biologically active polymeric coating
16.	<u>Krivova M.G.</u> , Savitskaya T.A., Grinshpan D.D.	Belarus	Modified carbon adsorbents for laundry waste water treatment
17.	<u>Lukashova M.S.</u> , Belikov K.N., Bryleva E.Yu., Grebnyuk N.N., Kalchenko V.I., Kharchenko S.G.	Ukraine	Sorption materials modified with functionalized thiakalixarenes for selective removal of Eu(III) from aqueous solutions
18.	<u>Gudyma Iu.V.</u> , <u>Maksymov A.Iu.</u>	Ukraine	The microscopic stochastic dynamics of spin-crossover coordination complexes
19.	<u>Mishurov D. O.</u> , Roshal A.D.	Ukraine	Synthesis and nonlinear optical properties of glycidyl derivatives of quercetin
20.	Samaryk V.Ja., <u>Nosova N.G.</u> , Tarnavchik I.T., Nagornyak M.I., Voronov S.A.	Ukraine	Synthesis of dicarboxylic α -amino-acids based polyesters via Steglich esterification
21.	<u>Opanasenko O.A.</u> , Sinelnikov S.I., Riabov S.V.	Ukraine	Sorption of methyl orange from water by crosslinked β -cyclodextrin-containing copolymers
22.	Kolosova O.S., Tatarets A.L., Obukhova O.M., Povrozin Ye.A., Khabuseva S.U., Sanin E.V., Terpetschnig E.A., <u>Patsenker L.D.</u>	Ukraine	A comparison of the molecular structure, properties and interaction with proteins of a series of fluorescent squaraine and nonsquaraine dyes

23.	Mahno S.M., Fatyeyeva K.Yu., Ratieuville V., Tarasyuk O.P., Chappey C., <u>Rogalsky S.P.</u>	Ukraine	Proton conducting membrane based on macroporous polyimide Matrimid® and protic ionic liquid
24.	<u>Roik N.V.</u> , Belyakova L.A., Dziazko M.O.	Ukraine	pH-controlled liberation of para-aminobenzoic acid from selectively functionalized MCM-41 silica
25.	<u>Semenova O.M.</u> , Obukhova O.M., Sanin E.V., Khabuseva S.U., Tatarets A.L., Jones G., Patsenker L.D.	Ukraine	Effect of iodine and bromine on the photophysical and photochemical properties of heptamethine indocyanine dyes and their protein conjugates
26.	<u>Sitnikov P.A.</u> , Ryabkov Y.I., Belykh A.G., Vaseneva I.N.	Russia	Influence of acid-base oxide surface properties on the reactivity of the epoxy compounds
27.	Kozitsky A.V., <u>Stroyuk O.L.</u> , Kuchmiy S.Ya., Klochko N.P., Klepikova K.S.	Ukraine	Photochemically-produced ZnO/CdS and ZnO/Cu ₂ S heterostructures based on electrodeposited zinc oxide films as electrodes of all-inorganic solar cells
28.	<u>Trofymchuk I.M.</u> , Belyakova L.A.	Ukraine	Silicas with supramolecular moieties for the selective removal of aromatic molecules
29.	<u>Vakaliuk A.V.</u> , Zaderko A.N., Grishchenko L.M., Bezugla T.M., Diyuk V.E.	Ukraine	Chemical properties of brominated activated carbon
30.	<u>Vasylets G.Y.</u> , Bukrinev A.S., Khotkevich A.V., Barszcz B., Starodub V.A.	Ukraine	Electroconductive TCNQ anion-radical salts with cations based on 3d-metals complexes
31.	<u>Yönetken Ahmet</u> , Erol Ayhan	Turkey	Investigation of electrical characteristics of composites produced by electroless Ni plating of SiC
32.	Çavdar Hamide, Erol Ayhan, <u>Yönetken Ahmet</u>	Turkey	Mechanical properties of a composite produced from electroless Ni plated WC and Ti powders
33.	<u>Yönetken Ahmet</u> , Erol Ayhan	Turkey	Production and characterization of implant material produced by using electroless ni plated Al ₂ O ₃ -Co-Cr-Ti powders
34.	<u>Chou Sheng-Ying</u> , Chen Yun	Taiwan	Synthesis, characterization and electron-injection application of copolymer based on benzimidazolyl and tetraethylene glycol ether

35.	<u>Malyovanyi S.M.</u> , Milovanova O.I., Panov E.V., Glushchak T.S.	Ukraine	Interaction of oxygen, low-molecular alcohols and ketones with doped SnO ₂ nanocrystals
36.	<u>Potapenko A.V.</u> , Panov E.V., Diamant V.A., Galaguz V.A.	Ukraine	Synthesis in salt melts and properties of a novel LiFePO ₄ – based cathodic material
37.	<u>Sakhno T.V.</u> , Barashkov N.N., Irgibayeva I.S., Aldongarov A.A., Mantel A.I.	Ukraine	Study of aggregation-induced emission of 5-(4-dimethylamino-benzyliden-barbituric acid and its use in fluorescent method of determining ethanol concentration in gasoline
38.	<u>Nifantiev K. S.</u> , Ischenko E. V., Byeda O. A.	Ukraine	Co-Ni/Al ₂ O ₃ methanation catalysts activity relation on Ni/Co ratio: an explanation approach based on reaction mechanism and kinetics
39.	<u>Aliyeva Z.M.</u> , Alverdiyev I.J., Bagheri S.M., Yusibov Yu.A., Babanly M.B.	Azerbaijan	Phase diagrams of the Ag ₈ GeX ₆ -Ag ₈ SnX ₆ (X-S, Se) systems and some properties of solid solutions
40.	<u>Rasulova K.D.</u> , Aliyev Z.S, Guliyeva U., Babanly M.B.	Azerbaijan	Phase equilibria in the YbTe-SnTe-Bi ₂ Te ₃ system
41.	<u>Imamaliyeva S.Z.</u> , Gasanyly T.M., Babanly M.B.	Azerbaijan	Phase equilibria in Tl ₅ Te ₃ -Tl ₉ SbTe ₆ -Tl ₉ LnTe ₆ (Ln-Sm, Gd) systems and some properties of solid solutions
42.	<u>Ünver H.</u> , Yıldız M., Kiraz A., Özgen Ö.	Turkey	Spectroscopic studies and structure of (Z)-6-[(2-hydroxyphenylamino)methylene]-2-methoxycyclohexa-2,4-dienone
43.	<u>Soldatkina L.M.</u> , Menchuk V.V.	Ukraine	Agricultural wastes/polyaniline nanocomposites as novel adsorbents for removal of anionic dyes from aqueous solutions