POSTER SESSION

July 14, 2004

A) Nanostructures and their Properties: Clusters, Nanotubes, and Quantum Dots

A1. Quantum-chemical simulation of $Y_2C_2@C_{82}$
A.N. Enyashin, Yu. N. Makurin, and A. L. Ivanovskii
Institute of Solid State Chemistry, Ural Branch of the RAS, Ekaterinburg, Russia

A2. Fe—S clusters: Applications to minerals and enzyme cofactors
M.R. Philpott[1], V. Kumar[2], and Y. Kawazoe[2]
[1]*National University of Singapore Department of Materials Science, Singapore*
[2]*Institute for Materials Research, Tohoku University, Sendai Japan*

A3. Research of nanoclusters size effect on the molecular-dynamic modeling results
E.I. Golovneva, I. F. Golovnev, and V.M. Fomin
Institute of Theoretical and Applied Mechanics, SB RAS, Novosibirsk, Russia

A4. Tight-binding simulation of optical absorption spectra FOR single-wall carbon nanotubes
P.N. Gevko, A.V. Okotrub, V.V. Belavin, and L.G. Bulusheva
Nikolaev Institute of Inorganic Chemistry, SB RAS, Novosibirsk, Russia

A5. The structure of H-bonded clusters in water and methanol in sub- and supercritical state
S.P. Krishtal[1], M.G. Kiselev[1], and V.V. Kislov[2]
[1]*Institute of Solution Chemistry, Russian Academy of Sciences, Ivanovo, Russia*
[2]*Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan*

A6. The modeling of Mo doped cylindrical and scroll-like V_2O_5 nanotube
V.V. Ivanovskaya, A.N. Enyashin, Yu.N. Makurin, V.L. Volkov, and A.L. Ivanovskii
Institute of Solid State Chemistry, UrB RAS, Ekaterinburg, Russia

A7. Heat capacities of buckministerfullerene
G.R. Vakili-Nezhaad and M. Hamedanian
NanoSciTech Research Center, University of Kashan, Kashan, Iran

A8. Design and topological properties of trivalent polyhedra as building units of inorganic materials
S F. Solodovnikov, V.I. Kosyakov, E.V. Grachev, V.Yu. Komarov, and A.Yu. Manakov
Nikolaev Institute of Inorganic Chemistry, SB RAS, Novosibirsk, Russia

A9. Molecular dynamics simulation of InGaAs/GaAs nanotubes
A.V. Bolesta, I.F. Golovnev, and V.M. Fomin
Institute of Theoretical and Applied Mechanics SB RAS, Novosibirsk, Russia

A10. Calculations on organic-solvent dispersion of single-wall carbon nanotubes
Francisco Torrens
Institut Universitari de Ciència Molecular, Universitat de València, València, Spain

A11. *Ab initio* molecular dynamics study of Cs-ion insertion and adsorption at cap and stem of carbon nanotubes

M. Khazaei, A.A. Farajian, H. Mizuseki, and Y. Kawazoe
Institute for Materials Research, Tohoku University, Sendai, Japan

A12. Computational Design of New Carbon Nanoclusters

D.V. Leshchev and S.V. Kozyrev
Center for Advanced Studies of the St. Petersburg State Polytechnical University, St. Petersburg, Russia

A13. Quantum-chemical investigations of the geometry and the energy structure of iron(II) and iron(III) hydroxoaquocomplexes

M.A. Popov[1], A.L. Ivanovskii[2], and D.G. Kleschev[1]
[1]*South-Urals State University, Chelyabinsk, Russia*
[2]*Institute of Solid State Chemistry, Ural Branch RAS, Ekaterinburg, Russia*

A14. Quantum-mechanics simulation of soot fragments and investigation of their activity in reactions with molecular oxygen

V.G. Zavodinsky, and Mikhailenko
Institute for Materials Science, Russian Academy of Sciences, Khabarovsk, Russia

A15. Molecular dynamics simulations of solid-liquid phase transition in small water aggregates

A.V. Egorov[1], E.N. Brodskaya[2], and A. Laaksonen[3]
[1]*Institute of Physics, St. Petersburg University, St. Petersburg, Russia*
[2]*Institute of Chemistry, St. Petersburg University, St. Petersburg, Russia*
[3]*Division of Physical Chemistry, Arrhenius Laboratory, Stockholm University, Stockholm, Sweden*

A16. Chemistry of nanodiamond surface

A.N. Yeremenko, O.A. Besedina, and I.I. Obraztsova
Kemerovo division of Institute of Solid State hemistry and Mechanochemistry, SB RAS, Kemerovo, Russia

A17. Computational geometry optimization of olygocalixarenes

E.V. Ostapova and H.N. Altshuler
Kemerovo division of Institute of Solid State Chemistry and Mechanochemistry, SB RAS, Kemerovo, Russia

A18. Open electronic states of embedded hydrogen atom in nanosystem

S.A. Beznosyuk, D.A. Mezentsev, V.A. Novozhenov, M.S. Zhukovsky, and T.M. Zhukovsky
Altai State University, Barnaul, Russian Federation

A19. Magnetic ordering in C_{60} polymers with partially broken intermolecular bonds

V.V. Belavin, L.G. Bulusheva, A.V. Okotrub
[1]*Nikolaev Institute of Inorganic Chemistry, SB RAS, Novosibirsk, Russia*

B) Nanostructures Formation and Characterization

B1. Numerical modeling of the coating property formation during electron-beam surfacing
A.G. Knyazeva, O.N. Kryukova, and N.V. Bukrina
Institute of Strength physics and material Science SB RAS, Tomsk, Russia

B2. Modelling of conditions of nanostructures forming during shock synthesis
V.N. Leitsin and M.A. Dmitrieva
Tomsk State University, Tomsk, Russia

B3. Influence of Schwoebel barrier and diffusion anisotropy on step density oscillation amplitude during epitaxy process
I.G. Neizvestny, N.L. Shwartz, and Z.Sh. Yanovitskaja,
Institute of Semiconductor Physics, SB RAS, Novosibirsk, Russia

B4. 100-nm MOSFET-gate formation by e-beam lithography
Yu.V. Nastaushev, VM. Kudryashov, F.N. Dultsev, T.A. Gavrilova, M.M. Kachanova, D.V. Sheglov, A.A. Franzusov, V.P. Popov, A.V. Latyshev and A.L. Aseev
Institute of Semiconductor Physics, SB RAS, Novosibirsk, Russia

B5. AFM tip-induced nano electro-mechanical surface modification
D.V. Sheglov, A.V. Latyshev, and A.L. Aseev
Institute of Semiconductor Physic,s SB RAS, Novosibirsk, Russia
Novosibirsk State University, Novosibirsk, Russia

B6. Gate dielectric based on TiO_2 for nanodevices
Yu.V. Nastaushev, O.V. Naumova, F.N. Dultsev, L.V. Litvin, M.M. Kachanova, D.V. Sheglov, VP. Popov, A.V. Latyshev, and A.L. Aseev
Institute of Semiconductor Physics, SB RAS, Novosibirsk, Russia

C) Materials Design and Properties Prediction

C1. New method for equation of state calculation of molecules adsorbed inside nanotubes and at their surfaces
A.S. Fedorov[1], P.B. Sorokin[1], A.A. Kuzubov[1], and S.G. Ovchinnikov[1,2]
[1]*Kirensky Institute of Physics, SB RAS, Krasnoyarsk, Russia*
[2]*UNESCO Faculty "New Materials and Technologies", Krasnoyarsk State Technical University, Krasnoyarsk, Russia*

C2. Excess of low-energy vibrational excitations in oxides: The specific heat anomalies as computed from density of states
A.I. Rykov[1], S. Kitao[2], T. Mitsui[3], A.P. Nemudry[4] and K. Nomura[1]
[1]*School of Engineering, University of Tokyo, Japan*
[2]*Research Reactor Institute, Kyoto University, Kyoto, Japan*
[3]*Japan Atomic Energy Research Institute, Hyogo, Japan*
[4]*Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia*

C3. Design of immobilized functional calixarenes via CS Chem3D program complex
H.N. Altshuler, E.V. Ostapova, and O.H. Altshuler
Kemerovo Division of Institute of Solid State Chemistry and Mechanochemistry, SB RAS, Kemerovo, Russia

C4. Ion-exchanger as canonic assembly
O.H. Altshuler and H.N. Altshuler
Kemerovo Division of Institute of Solid State Chemistry and Mechanochemistry, SB RAS, Kemerovo, Russia

C5. Computational and phenomenological classification and search of new acentric borate crystals for optoelectronics
V.V. Atuchin[1], B.I. Kidyarov[1], and N.V. Pervukhina[2]
[1]*Institute of Semiconductor Physics, SB RAS, Novosibirsk, Russia*
[2]*Nikolaev Institute of Inorganic Chemistry, SB RAS, Novosibirsk, Russia*

C6. MS XOMEGA and MS CONTINUOUS - program complex for calculations of the ground states and XANES spectra by full multiple scattering
Ph. Ruzankin
Boreskov Institute of Catalysis, SB RAS, Novosibirsk, Russia

C7. Thermo fluctuation phenomena in lithium niobate analysis
D.I. Shevtsov, I.S. Azanova, A.B. Volyntsev, A.E. Bachurin, and A. Lu
Perm State University, Perm, Russia

C8. The internal coordinates method to study potential energy surfaces
I.H. Umirzakov
Kutateladze Institute of Thermal Physics SB RAS, Novosibirsk, Russia

C9. Development of calculations models and methods describing the microdefect formation and distribution peculiarities during dislocation-free silicon large diameter single crystal growth
A.I. Prostomolotov and N.A. Verezub
Institute for Problems in Mechanics RAS, Moscow, Russia

C10. Collisional thermostat and its role for the creation of initial state and molecular dynamics simulations of complex molecular systems
N.K. Balabaev
Institute of Mathematical Problems of Biology RAS, Pushchino, Moscow region, Russia

C11. Computer projecting of technologies and materials with demanded properties
P.A. Vitiaz[1], O.V. Zhilinsky[2], and T.V. Laktyushina[3]
[1]*NASB, Minsk, Belarus*
[2]*Institute of Mechanics and Machine Reability, NASB, Minsk, Belarus*
[3]*Institute of Heat and Mass Transfer, NASB, Minsk, Belarus*

C12. A generalization of the tight-binding approach to binary liquid transition-metal alloys
N.E. Dubinin and N.A.Vatolin
Institute of Metallurgy of the UrB RAS, Ekaterinburg, Russia

C13. Using of wavelet analysis for parameterization and simulation of surface mesostructure of deformed metals

P.V. Kuznetsov[1], L.A. Bityutskaya[2], and Y.V. Bogatikov[2]
[1]*Institute of Strength Physics and Materials Science, SB RAS, Tomsk, Russia*
[2]*Voroneg State University , Voroneg, Russia*

C14. Search of porous crystal structures and prediction of possible host—guest complexes using new algorithms based on Voronoi-Dirichlet polyhedra

V.A. Blatov, A.P. Shevchenko, and A.V. Virovets
Nikolaev Institute of Inorganic Chemistry, SB RAS, Novosibirsk, Russia

C15. One aspect of chemico-thermodynamical modeling in solution of complex problems of describing the states for homo- and heterogeneous systems

A.P. Ryzhich, V.I. Belevantsev, V.I. Malkova, and B.S. Smolyakov
Nikolaev Institute of Inorganic Chemistry, SB RAS, Novosibirsk, Russia

C16. Generation algorithms and design of tetrahedral frameworks built from symmetrically equivalent polyhedra

V.Yu. Komarov, E.V. Grachev, S.F. Solodovnikov, A.Yu. Manakov
Nikolaev Institute of Inorganic Chemistry, SB RAS, Novosibirsk, Russia

C17. Numerical methods of modeling mesostructure of materials

R.M. Kadushnikov[1], E.Y. Nurkanov[2], V.M. Alievsky[2], and I.V. Antonov[2]
[1]*Smart Imaging Technologies Co, Houston, USA*
[2]*Ural State Technical University, Ekaterinburg, Russia*

C18. Structure of liquid alkali metals within the square-well model, and mean spherical approximation

N.E. Dubinin, V.V. Filippov, O.G. Malkhanova, and N.A. Vatolin
Institute of Metallurgy of the UrB RAS, Ekaterinburg, Russia

C19. Thermodynamic simulation of molten aluminum alloys

N.M. Barbin, G.K. Moiseev, N.I. Iljinikh, G.F. Kazantsev, N.A. Vatolin
Institute of High-Temperature Electrochemistry, UrB RAS

C20. Efficient procedure for view factors calculation in 2*d* axisymmetric geometries

Berdnikov V.S., Skoblikov S.V., Tokmakova O.V.
Kutateladze Institute of Thermophysics, SB RAS, Novosibirsk

C22. Solid solutions in the Sm(Nd)—Ba—Cu—O system: simulation of decomposition processes, peak-effect

N.I. Matskevich[1], T.D. Karpova[1], Yu.G. Stenin[1],
E.A. Trofimenko[2], Yu.D. Tretyakov[2], Th. Wolf[3]
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[3]*Institute of Solid State Physics, Karlsruhe Research Center, Karlsruhe, Germany*

C23. Account for relativistic effects in ices H_2O and D_2O: computer simulation of thermal anomalies

S.P. Gabuda, S.G. Kozlova
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C24. Magnetic properties hexanuclear clusters of K7Mo6Q8(CN)6.8H2O (Q = S, Se)

S.P. Gabuda, V.N. Ikorskii, S.G. Kozlova, Yu.V. Mironov, V.E. Fedorov
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C25. Excided state in hexanuclear chalcocyanide rhenium clusters

S.G. Kozlova, S.P. Gabuda, K.A. Brylev, Yu.V. Mironov, V.E. Fedorov
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July 15, 2004

Computational Materials Solids, Condensed matter

D) Structural, Electronic and Dynamical Properties

D1. Computation of interatomic voids in complex molecular systems

M.G. Alinchenko[1], N.N. Medvedev[1] , A.V. Anikeenko[1],
V.P. Voloshin[1], M.L. Gavrilova [2], and P. Jedlovszky[3]
[1]*Institute of Chemical Kinetics and Combustion, SB RAS, Novosibirsk, Russia*
[2] *Department of Computer Science, University of Calgary, Calgary, AB, Canada*
[3]*University of Budapest, Hungary*

D2. Classical and *ab initio* simulation of the liquid metals

Yu. Mitrokhin
Udmurt State University, Izevsk, Russia

D3. DFT investigation of impurities in silicon carbide

E.I. Yuryeva
Institute of Solid State Chemistry, UrB RAS, Ekaterinburg, Russia

D4. *Ab initio* modeling of Ge behaviour in PbTe semiconductor

A.S. Zyubin[1], S.N. Dedyulin[2], and V.I. Shtanov[2]
[1]*Institute of Problems of Chemical Physics RAS, Chernogolovka, Moscow Region, Russia*
[2]*Department of Chemistry, Moscow State University, Moscow, Russia*

D5. Lithium ion quadrupolar relaxation in aqueous solutions. A molecular dynamics simulation study

A.V. Egorov[1], V.I. Chizhik[1], A.P. Luybartsev[2], and A. Laaksonen[2]
[1]*Institute of Physics, St. Petersburg University, St. Petersburg, Russia*
[2]*Division of Physical Chemistry, Arrhenius Laboratory, Stockholm University, Stockholm, Sweden*

D6. Cation distribution and magnetic structure in brownmillerite Ca_2FeMnO_5

A.I. Rykov[1], T. Mitsui[2], A.P. Nemudry[3], K. Nomura[1],
Yu.T. Pavlyukhin[3], M. Tokunaga[4], and X. Zhang[5]
[1]*School of Engineering, The University of Tokyo, Tokyo, Japan*
[2]*Japan Atomic Energy Research Institute, Hyogo, Japan*
[3]*Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia*
[4]*Department of Applied Physics, The University of Tokyo, Tokyo, Japan*
[5]*High Energy Accelerator Research Organization, Photon Factory, Tsukuba, Japan*

D7. The investigation of bulk and surface electronic structure group III− V semiconductors

S.E. Kulkova[1], A.V. Subashiev[2], and D.V. Khanin[1]
[1]*Institute of Strength Physics and Materials Science of RAS, Tomsk, Russia*
[2]*St. Petersburg State Technical University, St. Petersburg, Russia*

D8. Structural polymorphism of the coordination compounds

N.V. Podberezskaya, G.V. Romanenko, N.V. Pervukhina, I.A. Baidina,
A.V. Virovets, C.A. Gromilov, V.I. Alekseev, C.V. Borisov, and V.V. Bakakin
Nikolaev Institute of Inorganic Chemistry, SB RAS, Novosibirsk, Russia

D9. Molecular dynamics simulation of lithium nucleus quadrupolar relaxation in aqueous solutions

A.V. Egorov[1], V.I. Chizhik[1], A.P. Luybartsev[2], and A.Laaksonen[2]
[1]*Institute of Physics, St. Petersburg University, St. Petersburg, Russia*
[2]*Division of Physical Chemistry, Arrhenius Laboratory, Stockholm University, Stockholm, Sweden*

D10. Electronic structure of 18-K superconductor Y_2C_3 and other yttrium carbides

I.R. Shein
Institute of Solid State Chemistry, UrB RAS, Ekaterinburg, Russia

D11. Band structures in superconducting AlB_2-like (Ca,Sr,Ba)Ga_xSi_{2-x}

I.R. Shein , N.I. Medvedeva, and A.L. Ivanovskii
Institute of Solid State Chemistry, UrB RAS, Yekaterinburg, Russia

D12. Conductivity calculation of liquid cesium in a wide temperature range

A.N. Sobolev, A.G. Vorontsov, and A.A. Mirzoev
South Ural State University, Chelyabinsk, Russia

D13. The strain simulation in proton exchange layers on the lithium niobate

I.F. Taisin, D.I. Shevtsov, I.S. Azanova, and A.B. Volyntsev
Perm State University, Perm, Russia

D14. Molecular dynamical studies of the detonation of a diatomic molecular crystal

A.V. Utkin, I.F. Golovnev, and V.M. Fomin
Institute of Theoretical and Applied Mechanics, SB RAS, Novosibirsk, Russia

D15. Vibrational spectra of KPb_2Cl_5 and KPb_2Br_5 crystals

A.N. Vtyurin[1], L.I. Isaenko[2], S N. Krylova[1],
A. Yelisseyev[2], A.P. Shebanin[2], and N.G. Zamkova[1]
[1]*Kirensky Institute of Physics, 660036 Krasnoyarsk, Russia*

[2]*Joint Institute of Geology, Geophysics and Mineralogy, Novosibirsk, Russia*

D16. The software package for interpretation of IR and Raman spectra of polyatomic molecules

V. Baltakhinov

Boreskov Institute of Catalysis, SB RAS, Novosibirsk, Russia

D17. The electronic structure and properties of rutile-type compounds $Sn_{1-x}M_xO_2$, M = As, Sb, Bi, V, Nb, Ta ($0 \le x \le 0.25$)

V.M. Zainullina

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D18. Condensed excited states in beryllium

V.A. Popov

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D19. Fermi surface of doped lithium

V.A. Popov

Altai State Technical University, Barnaul, Russia

D20. Electron momentum density, inter-atomic interaction and phase stability B2 Ti-transition metals intermetallics

A.A. Baturin and A.I. Lotkov

Institute of Strength Physics and Material Science, SB RAS, Tomsk, Russia

D21. Symmetry analysis of calculated vibrational spectra of Rb_2KScF_6 crystal

A.S. Krylov[1], A. Bulou[2], S.N. Krylova[1], V.N. Voronov[1], A.N. Vtyurin[1], and N.G. Zamkova[1]

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[2]*Universite du Maine, Le Mans, France*

D22. Account of three-particle interactions in lattice dynamics method

D.S. Krupskiy, O.S.Subbotin, V.R. Belosludov

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D23. Crystal chemistry of metal hypophosphites and structural base for some physicochemical properties

D.Y. Naumov, M.I. Naumova, N.V. Kuratieva, and N.V. Podberezskaya

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D24. Nucleation Mechanisms of Clathrate Silicates (Clathrasils)

A.A. Pomeransky

Nikolaev Institute of Inorganic Chemistry, SB RAS, Novosibirsk, Russia

E) Thermodynamics Properties of Materials

E1. Thermodynamics and kinetic of multi-barrier formation of crystal nucleus in the liquid

B.I. Kidyarov, and A.B. Meshalkin

Institute of Thermophysics SB RAS, Novosibirsk, Russia

E2. The structures with sublattices of vacancies (design and thermodynamic stability)
V.I. Kosyakov and V.A. Shestakov
Nikolaev Institute of Inorganic Chemistry SB RAS, Novosibirsk, Russia

E3. Kinetics of hydrites decomposition in nonisothermal conditions
L.G. Malyshev
The Urals State Technical University USTU-UPI, Ekaterinburg, Russia

E4. Modeling of the condensation process in $ZrOCl_2*8H_2O$ solution
N.V. Mezentseva[1], V.A. Sadykov[2], and V.L. Kuznetsov[2]
[1]*Novosibirsk State University, Novosibirsk, Russia*
[2]*Boreskov Institute of Catalysis, SB RAS, Novosibirsk, Russia*

E5. Dynamical and thermodynamical properties of hydrogen clathrate at different cage occupation
T.M. Inerbaev[1,2], V.R. Belosludov[1,2], R.V. Belosludov[1,2], M. Sluiter[1], and Y. Kawazoe[1]
[1]*Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan*
[2]*Nikolaev Institute of Inorganic Chemistry, SB RAS, Novosibirsk, Russia*

E6. The free energy of disordered solid solution
V.A. Krashaninin
Institute of Metallurgy, Ural Branch RAS, Ekaterinburg, Russia

E7. Thermodynamics and vibration spectra for molecular crystals of beta-diketonates of metals: Modelling in frameworks of the lattice dynamics method
V.N. Naumov, N.A.Nemov, G.I. Frolova,
V.R. Belosludov, M.A. Bespyatov, and I.K. Igumenov
Nikolaev Institute of Inorganic Chemistry, SB RAS, Novosibirsk, Russia

E8. Crystal theremal conductivity influence on his convective heat transfer with the surroundings during czochralski growth
V.S. Berdnikov, A.M. Grigorieva, Yu.L. Zandanova
Institute of Thermophysics, SB RAS, Novosibirsk, Russia

E9. Thermodynamic model of inverse melting in Titanium binary alloys
S. Ranganathan[1] and P. Ramachandra Rao[2]
[1]*National Metallurgical Laboratory, Jamshedpur, India*
[2]*Banaras Hindu University, Varanasi, India*

E11. Mixed convection flow of the melt and heat transfer in a czochralski motionless crucible
V.S. Berdnikov, V.A. Vinokurov, V.V. Vinokurov, V.A. Gaponov
Institute of Thermophysics, SB RAS Novosibirsk, Russia

F) Interaction on Surfaces and Interfaces

F1. Experimental and theoretical investigation of PbTe(100) oxidation in dry oxygen

E.V. Tikhonov[1], T.S. Zyubina[2], S.P. Kobeleva[3], V.S. Neudachina[1], and L.V. Yashina[1]
[1]*Department of Chemistry, Moscow State University, Moscow, Russia.*
[2]*Institute of Problems of Chemical Physics RAS, Chernogolovka, Moscow Region, Russia.*
[3]*State Institute for Rare Metals, Moscow, Russia*

F2. The electronic structure of grain boundary in nickel

S.V. Eremeev and S.E. Kulkova
Institute of Strength Physics and Materials Science, Tomsk, Russia

F4. Theoretical study of surface electronic structure and hydrogen adsorption properties in advanced hydrogen storage materials

S.E. Kulkova[1], D.I. Bazhanov[2], S.V. Eremeev[1], and D.V. Chudinov[1]
[1]*Institute of Strength Physics and Materials Science, SB RAS, Tomsk, Russia*
[2]*Moscow State University, Moscow, Russia*

F5. Electron-microscopic researches of various external influences on thin films C_{60}

V. Rahvalov[1] and D. Spoiala[2]
[1]*Institute of Applied Physics, Academy of Science of Moldova, Moldova*
[2]*State University of Moldova, Moldova*

F6. Theoretical study of the adsorption of metal atoms on metallic surfaces

A.V. Matveev, M.V. Mamonova, and V.V. Prudnikov
Omsk State University, Omsk, Russia

F7. *Ab initio* study of the interaction of PbX(X = S, Te) surfaces with oxygen

T.S. Zyubina[1], V.S.Neudachina[2], L.V. Yashina[2], and V.I. Shtanov[2]
[1]*Institute of Problems of Chemical Physics RAS, Chernogolovka, Moscow Region, Russia*
[2]*Department of Chemistry, Moscow State University, Moscow, Russia*

F8. Austenite and martensite TiNi surface electronic structure and metal-insulator transition under oxide layers growth

S.E. Kulkova, V.E. Egorushkin, and S.V. Eremeev
Institute of Strength Physics and Materials Science, Tomsk, Russia

F9. Reactivity of ultradispersed diamonds

D. Karpalerv and O. Efimov
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G) Microstructure and its Physical and Chemical Properties

G1. The influence of intensive cold rolling in martensitic transformations and shape memory effect in TiNi-based alloys

A.I. Lotkov, E.F. Dudarev, E.D. Kudinova, V.N. Grishkov, T.Yu. Maletkina
Institute of Strength Physics and Materials Science SB RAS, Tomsk Russia, Siberian Physico-Technical Institute, Tomsk State University, Tomsk, Russia

G2. The structure of lead-silicate glasses: Molecular dynamics and XPS studies

O.M. Kanunnikova[1], A. Kimmel[1], and I.L. Lomaev[2], I.N. Gusenkov[1]
[1]*Physical-Technical Institute, Izevsk, Russia*
[2]*Udmurtian State University, Izevsk, Russia*

G3. Eutectic line for the metastable freezing binary systems

M.P. Anisimov and A.V. Illarionov
Boreskov Institute of Catalysis, SB RAS, Novosibirsk, Russia

G4. *Ab initio* study of the softening and hardening effects in bcc alloys

N.I. Medvedeva[1] and Yu.N. Gornostyrev[2]
[1]*Institute of Solid State Chemistry, Ekaterinburg, Russia*
[2]*Russia Institute of Metal Physics, Ekaterinburg, Russia*

G5. Grain boundary sliding and migration in copper: Effect of vacancy

P. Ballo[1], V. Slugen[2], and G. Farkas[2]
[1]*Department of Physics, Faculty of Electrical Engineering and Information Technology, Slovak University of Technology, Bratislava*
[2]*Department of Nuclear Physics and Technology, Faculty of Electrical Engineering and Information Technology, Slovak University of Technology, Bratislava*

G5. Simulation of motion dislocation under stochastic external influences

A.B. Volyntsev and A.V. Ratt
Perm State University, Perm, Russia

G6. First-principles efficient pair potentials in alloys of the simple metals

V.A. Krashaninin and C.C. Alexandrova
Institute of Metallurgy, Ural Branch RAS, Ekaterinburg, Russia

G7. Physicochemical properties of ultradispersed copper powders

I.I. Obraztsova and G.Y. Simenyuk
Kemerovo Division of Institute of Solid State Chemistry and Mechanochemistry, SB RAS, Kemerovo, Russia

G8. Modeling of the structure and vibrational properties of LDA, HDA and VHDA

O.S. Subbotin[1], V.R.Belosludov[1], T.M. Inerbaev[1,2], R.V. Belosludov[1,2] and Y. Kawazoe[2]
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G9. Optical response in disordered alloys

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G10. Simulation of conditions of realization of synthesis processes in shock-loaded powder Ti-C type

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