Second Conference of the Asian Consortium for Computational Materials Science (ACCMS-2)
July 14-16, 2004, Novosibirsk, Russia
House of Scientists in Novosibirsk Scientific Centre

CONFERENCE PROGRAM

July 14, 2004

9:00-17:00 **Registration**

9:45 **Opening Ceremony**

Opening Addresses
Prof. F.A. Kuznetsov
Nikolaev Institute of Inorganic Chemistry SB RAS, Novosibirsk, Russia
Prof. Y. Kawazoe
Institute for Materials Research, Tohoku University, Sendai Japan

Session I **Materials Design from First Principles: Novel Nanostructured Materials**
Chairs: Prof. F. A. Kuznetsov, Russia / Prof. S. de Leeuw, Holland

10:00 **Ultimate *ab initio* calculations to predict new materials expected to be used in nanotechnology**
Y. Kawazoe
Institute for Materials Research, Tohoku University, Sendai, Japan

10:45 **Novel properties of matter at the nanoscale in mixed systems**
V. Kumar
Institute for Materials Research, Tohoku University, Sendai, Japan & VKF, Chennai, India

11:10 **Coffee break**

Session II **Physical Properties of Materials**

Chairs: Prof. Y. Kawazoe, Japan / Prof. A. L. Ivanovskii, Russia

11:30 **Operating experience on creating databases of inorganic materials**
A. A. Titov, V. A. Titov, L. I. Chernyavskii, and F. A. Kuznetsov
Nikolaev Institute of Inorganic Chemistry, SB RAS, Novosibirsk, Russia

11:55 **A correlation between structure, energy and molar volume of the polyhedric**
V. I. Kosyakov, V. Yu. Komarov, E. V. Grachev, A. V. Kurnosov, V. A. Shestakov, and S. F. Solodovnikov
Nikolaev Institute of Inorganic Chemistry, SB RAS, Novosibirsk, Russia

12:20 **Pyroelectric vector as a novel measure of crystal polarity**
E. V. Kholopov
Nikolaev Institute of Inorganic Chemistry, SB RAS, Novosibirsk, Russia

12:45 **A first principles study of hardness in perovskite-type rare earth rhodium borides and carbides**

R. Sahara[1], T. Shishido[1], V. Kumar[1,2], and Y. Kawazoe[1]
[1]*Institute for Materials Research, Tohoku University, Sendai, Japan.*
[2]*Dr. Vijay Kumar Foundation, Chennai, India*

13:00-14:15 **Lunch break**

Session III — Clusters and Fullerenes

Chairs: Prof. H. Mizuseki, Japan / Prof. A. V. Okotrub, Russia

14:20 **Theoretical study of polarons and self-trapped excited states in one-dimensional C_{60} crystal**

V. R. Belosludov[1], T. M. Inerbaev[1,2], R. V. Belosludov[1,2], Y. Kawazoe[2], and J. Kudoh[3]
[1]*Nikolaev Institute of Inorganic Chemistry, SB RAS, Novosibirsk, Russia*
[2]*Institute for Material Research, Tohoku University, Sendai, Japan*
[3]*Center for Northeast Asia Studies of Tohoku University, Sendai, Japan*

14:45 **Diffusion monte carlo study on TM@Si_n (TM=Ti, Cr ; n=5-16)**

R. Maezono[1], K. Hongo[2], H Kawamura[2], V. Kumar[2], Y. Kawazoe[2], and H. Yashuhara[2]
[1]*National Institute for Materials Science, Computational Materials Science Center, Tsukuba, Japan,*
[2]*Instutute for Materials Research, Tohoku University, Sendai, Japan*

15:00 ***Ab initio* study of dititaniym endofullerens $Ti_2@C_{80}$**

A. N. Enyashin, Yu. N. Makurin, and A. L. Ivanovskii
Institute of Solid State Chemistry, Ural Branch of the RAS, Ekaterinburg, Russia

15:15 **Design for UV-cut materials made of novel silicon oligomers**

M. Takahashi and Y. Kawazoe
Institute for Materials Research, Tohoku University, Sendai, Japan

15:30 **Coffee break**

Session IV — Surfaces and Interfaces I

Chairs: Prof. Z. Sh. Yanovitskaya, Russia / Prof. V. Kumar, Japan / India

15:50 **First principles study of copper/alumina and gold/titania interfaces: effects of interface stoichiometry**

M. Kohyama[1], S. Tanaka[1], K.Okazaki[1], R. Yang[1], and Y. Morikawa[2,3]
[1]*Materials Science Research Group, Research Institute for Ubiquitous Energy Devices, National Institute of Advanced Industrial Science and Technology,, Osaka , Japan*

[2] *Research Institute for Computational Science, National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan*
[3] *Institute of Science and Industrial Research, Osaka University, Osaka Japan*

16:15 **Structural forms of two-valent metal cation stabilization in high-zeolite. The possibility of appearing of unusually active sites**
G. M. Zhidomirov
Boreskov Institute of Catalysis, Novosibirsk, Russia

16:40 **Monte Carlo simulation of ALD processes on flat and rough substrates**
I. G. Neizvestny, N. L. Shwartz, Z. Sh.Yanovitskaya, and A.V. Zverev
Institute of Semiconductor Physics SB RAS, Novosibirsk, Russia

17:00-19:00 **Poster Session**

July 15, 2004

9:00 - 17:00 **Registration**

Session V **Modeling of Disordered Systems and Defects in Materials**

Chairs: Prof. G. P. Das, India / Prof. S. E. Kulkova, Russia

09:00 **Beyond the point defect limit: simulation approaches to solid solutions and highly disordered systems**
N. L. Allan
School of Chemistry, University of Bristol, Bristol, UK

09:25 **Prediction of the thermopower and rational design of high efficiency thermoelectric materials based on low band gap crystalline polymers**
X. Gao and J. S. Tse
Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa Ontario, Canada

09:40 **Atomistic simulations of surface diffusion and segregation in ceramics**
M. Yu. Lavrentiev[1], N. L. Allan[1], J. H. Harding[2], D. J. Harris[2], and J. A. Purton[3]
[1] *School of Chemistry, University of Bristol, Bristol, UK*
[2] *Department of Physics and Astronomy, University College London, London, UK*
[3] *Daresbury Laboratory, Cheshire, UK*

09:55 **Atomistic simulation of the influence of pressure on the nucleation of dislocation in bcc Mo**

D. S. Xu[1], R. Yang[1], J. Li[2], J. P. Chang[3], and S. Yip[3]
[1] *Titanium Alloy Laboratory, Institute of Metal Research, Chinese Academy of Sciences, Shenyang, China*
[2] *Department of Materials Science and Engineering, Ohio State University, Columbus, USA*
[3] *Department of Nuclear Engineering, Massachusetts Institute of Technology, Cambridge, USA*

10:10 **Coffee break**

Session VI — Modeling of Ionic Materials

Chairs: Prof. V.M. Tapilin, Russia / Prof. K. Ohno, Japan

10:30 ***Ab initio* calculations of physical properties of ionic crystals**

E. G. Maksimov,
P.N. Lebedev Physical Institute, RAS, Moscow, Russia

10:55 **First principles simulation of electrode materials**

S. de Leeuw
DelftChemTech, Delft University of Technology, Delft, Holland

11:20 **Sructural and electronic properties of group IV phosphides and nitrides**

Y. P. Feng, M. Huang, A. T.-L. Lim, and F. Ding
Department of Physics, National University of Singapore, Singapore
Zheng Center for Data Intensive Computing, Brookhaven National Laboratory, Upton, USA

11:45 **Molecular dynamics simulation of fluorite- and tysonite-type solid electrolytes**

I. Yu. Gotlib, E. M. Piotrovskaya, and I. V. Murin
St.Petersburg State University, St.Petersburg, Russia

12:00 **Bond ionicity and its application on solids**

Z. Wu
Key Laboratory of Rare Earth Chemistry and Physics, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun, China

12:15 **First-principles calculations of the electronic structure and properties of $Ni_{1-x}Li_xO_{1-y}$ (0 £ x £ 1/4; 0 £ y £ 1/8) by LSDA+U.**

V. M. Zainullina[1], M. A. Korotin[2], Yu. P. Zaikov[3], and N. I. Shurov[3]
[1]*Institute of Solid State Chemistry, Ural Branch RAS, Ekaterinburg, Russia*
[2]*Institute of Metal Physics, Ural Branch RAS, Ekaterinburg, Russia*
[3]*Institute of Hightemperature Electrochemistry, Ural Branch RAS, Ekaterinburg, Russia*

12:30 **Stuctural properties and lattice dynamics of $RbMnCl_3$ crystal**

A. N. Vtyurin[1], S. A Goryainov[2], N. G. Zamkova[1], V. I. Zinenko[1], A. S. Krylov[1], and S. N. Krylova[1]
[1]*Kirensky Institute of Physics, Krasnoyarsk, Russia*
[2]*Joint Institute of Geology, Geophysics and Mineralogy,SB RAS, Novosibirsk,*

Russia

12:45-14:00 **Lunch break**

Session VII **Spintronics and Magnetic Materials**
Chairs: Prof. G. M. Zhidomirov / Prof. Z. Wu, China

14:05 **Dilute magnetic semiconductor spintronics materials: A first-principles approach**
G. P. Das
TPPED, Bhabha Atomic Research Centre, Mumbai, India

14:30 **Magnetic interactions in molecular magnets from first-principles calculation**
A. Postnikov
Institute of Metal Physics, Russian Academy of Sciences, Yekaterinburg, Russia; Osnabrück University - Department of Physics, Osnabrück, Germany

14:55 **First principles study of novel magnetic materials**
I. Dasgupta
Department of Physics and Meteorology, Indian Institute of Technology Kharagpur, Kharagpur & Department of Physics, Indian Institute of Technology Powai, Mumbai, India

15:20 **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*

15:35 **Designing electronic properties of transition-metal oxides**
I. Solovyev
PRESTO-JST, Institute for Solid State Physics, University of Tokyo, Japan

15:50 **Magnetic ordering in C_{60} polymers with partially broken intermolecular bonds**
V. V. Belavin, L.G. Bulusheva, A.V. Okotrub
Nikolaev Institute of Inorganic Chemistry, SB RAS, Novosibirsk, Russia

16:10-18:10 **Poster Session**

18:30 **Banquet**

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Session IX **New Approaches for Materials Design and Properties Predictions**
Chairs: Prof. T. Ikeshoji, Japan / Prof. V. G. Zavodinsky, Russia

09:00 **Development of integrated nanosimulation system and its applications**
M. Mikami
Research Institute for Computational Sciences (RICS)
National Institute of Advanced Industrial Science and Technology (AIST)
Umezono, Tukuba , Japan

09:25 **Time saving techniques for electronic structure calculation of infinite and semi-infinite crystals, interfaces and slabs of arbitrary thickness**

V. M. Tapilin
Boreskov Institute of Catalysis ,SB RAS, Novosibirs, Russia

09:50 **Expansion of unrestricted determinants in the basis of paired orbitals**
I. Zilberberg
Boreskov Institute of Catalysis, Novosibirsk, Russia

10:05 **Complex chemical bond method: theory and applications**
Z. J. Wu and S. Y. Zhang
Key Laboratory of Rare earth Chemistry and Physics
Changchun Institute of Applied Chemistry Chinese Academy of Sciences
Changchun ,China

10:20 **Coffee break**

Session X

Molecular Dynamics, Monte-Carlo and Multiscale Modelling of Materials

Chairs: Prof. E. G. Maksimov, Russia / Prof. J. Ihm, Korea

10:40 **First Principles Molecular Dynamics Simulation of Super Critical Water and Aqueous Solutions**
T. Ikeshoji
Research Institute for Computational Sciences (RICS)
National Institute of Advanced Industrial Science and Technology (AIST)
Tsukuba, Japan

11:05 **Multi-scale modeling of materials for fusion power plants**
D. Nguyen-Manh
Theory and Modelling Department, UKAEA, Culham Science Centre, Oxfordshire, UK

11:30 **Molecular dynamics simulation of the single wall nanotube growth**
K. Esfarjani and N. Gorjizadeh
Department of Physics, Sharif University of Technology, Tehran, Iran

11:55 **Nuclear Analysis of the Copper Alloys for Fusion Technologies by Monte Carlo Method**
G. Farkas[1], P. Domonkoš[2], V. Slugeò[2], P. Ballo[3], M. Greschner[4]
[1]*Department of Power Engineering,*
[2]*Department of Nuclear Physics and Technology,*
[3]*Department of Physics, Faculty of Electrical Engineering and Information Technology, Slovak University of Technology, Bratislava, Slovakia*
[4]*Institut für Kern- und Teilchenphysik, Technische Universität Dresden, Dresden, Germany*

12:10 **Application of Propagator Modification of Molecular Dynamic Method for Investigation of the processes of phthalocyanine films growth**
I. Golovnev[1], T. Basova[2], E. Kol'tsov[2], N. Alexandrova[1], and I. Igumenov[2]
[1]*Institute of Theoretical and Applied Mechanics, SB RAS, Novosibirsk, Russia*
[2]*Nikolaev Institute of Inorganic Chemistry, SB RAS, Novosibirsk, Russia*

12:25 **Molecular dynamics computer simulations of unsaturated phospholipid, and mixed phospholipid/cholesterol menbranes**
A. L. Rabinovich[1], P. O. Ripatti[1], and N. K. Balabaev[2]
[1]*Institute of Biology, Karelian Research Centre, RAS, Petrozavodsk Russia*
[2]*Institute of Mathematical Problems of Biology, Russian Academy of Science, Pushchino, Moscow Region, Russia*

12:40-13:45 **Lunch break**

Session XI **Molecular Nanoelectronics**

Chairs: Prof. J. Tse, Canada / Prof. V. L. Kuznetsov, Russia

13:50 **Nonequilibrium charge transport through single organic molecules**
J. Ihm
School of physics, Seoul National University, Seoul, Korea

14:15 **First principles calculations of optical absorption spectra of atoms in the vacuum and crystals**
K. Ohno[1], M. Furuya[1], Y. Noguchi[1], S. Ishii[1,2], and Y. Kawazoe[2]
[1]*Department of Physics, Yokohama National University, Yokohama, Japan*
[2]*Institute for Materials Research, Tohoku University, Sendai, Japan*

14:40 **Realization of molecular and atomic interconnection for molecular electronics: Theoretical aspects**
R. V. Belosludov[1,2], A. A. Farajian[1], Y. Kikuchi[1], H. Mizuseki[1] and Y. Kawazoe[1]
[1]*Institute for Materials Research, Tohoku University, Sendai, Japan*
[2]*Nikolaev Institute of Inorganic Chemistry, SB RAS, Novosibirsk, Russia*

15:00 **Special Session**

Chairpersons: Prof. K. Yamada, Prof. F. A. Kuznetsov, Prof. Y. Kawazoe

Greetings from **Prof. Takashi Yoshimoto**, President of Tohoku University, Sendai, Japan

15:20-15:40 **Coffee break**

Continuation of Session XI **Molecular Nanoelectronics**

Chairs: Prof. J. Tse, Canada / Prof. V. L. Kuznetsov, Russia

Ultra-fast designing of functional materials for molecular devices by first

15:40 **principles and genetic algorithm**

H. Mizuseki, N. Igarashi, R. V. Belosludov, A. A. Farajian, and Y. Kawazoe
Institute for Materials Research, Tohoku University, Sendai, Japan

15:55 **Ballistic conductance of magnetic nanowires**

A. Smogunov[1,2,3], A. Dal Corso[1,2], and E. Tosatti[1,2,4]
[1] *SISSA, 34014 Trieste, Italy*
[2] *INFM, 34014 Trieste, Italy*
[3] *Voronezh State University,Voronezh, Russia*
[4] *ICTP, 34014, Trieste, Italy*

Session XII — Surfaces and Interfaces II

Chairs: Dr. I. Zilberberg, Russia / Prof. N. Duc, UK

16:10 **Ta Deposition on Ta(100) Using Monte Carlo Method**

J. S. Tse
Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa, Canada

16:35 ***Ab initio* study on the carbon incorporation into the Si(001) surface**

H. Kim,
Div. of Chemical Metrology and Materials Evaluation Korea Research Institute of Standards and Science, Yuseong, Daejeon, Korea

17:00 **Kinetic Role of Surfactants in Nanowire Formation on Si(100)**

J. Wang[1], D. Wang[1], E. Wang[1], H. Mizuseki[2], Y. Kawazoe[2], M. Naitoh[3], and S. Nishigaki[3]
[1] *Institute of Physics, Chinese Academy of Sciences, Beijing, China*
[2] *Institute for Materials Research, Tohoku University, Sendai,, Japan*
[3] *Department of Electrical Engineering, Kyushu Institute of Technology, Kitakyushu, Japan*

17:25 ***Ab initio* simulation of diamond epitaxial growth on copper**

V. G. Zavodinsky
Institute for Materials Science, RAS, Khabarovsk, Russia

17:40 **First principles calculations of half-metallic zinc-blende type superlattices**

M. Geshi[1], M. Shirai[2], K. Kusakabe[1], and N. Suzuki[1]
[1]*Graduate School of Engineering Science, Osaka University, Osaka, Japan*
[2]*Research Institute of Electrical Communication, Tohoku University, Sendai, Japan*

17:55 **Specific aspects of silicon carbide whiskers nucleation on the surface of liquid metal particle**

I. N. Mazov[1] and V. L. Kuznetsov[2]
[1]*Novosibirsk State University, Novosibirsk,Russia*
[2]*Boreskov Institute of Catalysis, SB RAS, Novosibirsk, Russia*

18:10 **Closing of conference**