



**Second Conference of the Asian Consortium for Computational Materials Science
(ACCMS-2)**

July 14-16, 2004, Novosibirsk, Russia

NIKOLAEV
INSTITUTE
OF INORGANIC
CHEMISTRY



Organized by

Nikolaev Institute of Inorganic Chemistry SB RAS,
Boreskov Institute of Catalysis SB RAS,
Institute of Semiconductor Physics SB RAS,
Kutateladze Institute of Thermal Physics SB RAS



Sponsors:

Russian Foundation for Basic Research,
Japan Technos,
Ministry of Industry, Science and Technologies of RF,
Siberian Branch of Russian Academy of Science,
Center for Northeast Asia Studies of Tohoku University, Sendai, Japan,
Asia-Pacific Academy of Materials (APAM)

**Second CIRCULAR
IMPORTANT INFORMATION**

We are glad to invite you to participate in the Second Conference of the Asian Consortium for Computational Materials Science (ACCMS-2), which will be organized in Novosibirsk (Akademgorodok) Russia during July 14-16, 2004. The first conference ACCMS-1 was held in Bangalore, India in November 2001.

The Asian Consortium for Computational Materials Science (<http://www-lab.imr.edu/~accms/>) has been set up to nurture and promote research and developmental activities in computational materials science in Asian countries. Computational materials science has emerged as a distinct multidisciplinary branch of science whose relevance and importance has come from (a) the desire to have a microscopic understanding of complex materials and phenomena, (b) the need to design novel materials with a desired combination of physical, chemical and metallurgical properties, and (c) the possibility to describe the basic inter-atomic interactions in materials via appropriate quantum mechanical and statistical mechanical tools. With the unprecedented growth of computer power and the developments of efficient and smart algorithms and codes, it is now possible to do large scale simulations of real materials with increasing complexity. A synergy amongst a wide variety of disciplines such as physics, chemistry, metallurgy, geology, biology, computer science and information technology is gradually coming to a reality due to advances in computer simulations. The Conference will emphasize all aspects of computational materials science.

ORGANIZER

The Conference is organized by the Nikolaev Institute of Inorganic Chemistry of Siberian Branch of Russian Academy of Sciences (SB RAS), Boreskov Institute of Catalysis SB RAS, Institute of Semiconductor Physics SB RAS, and Kutateladze Institute of Thermal Physics SB RAS (Novosibirsk, Russia).



VENUE

The Conference will be held at the Novosibirsk Scientific Centre (Akademgorodok). The scientific program will start on Wednesday morning, July 14, and the last scientific session is scheduled on Friday evening, July 16.

Akademgorodok is the capital of Siberian Science (we invite you to visit the web site <http://www.sbras.ru/eng/welcome.html>) and accounts for about a half of the Division's research potential (22 research institutes in natural, technical and social sciences). Situated 30 km far from Novosibirsk city, it is a large industrial, scientific and cultural centre of Russia, in the beautiful forest. Akademgorodok is an interesting place not only for the scientific activities, but also for leisure.



The Conference will be located in the House of Scientists in Novosibirsk Scientific Centre.

LANGUAGE

English will be the official Conference language.

SCIENTIFIC PROGRAM

The deliberations of the ACCMS -2 will cover topics such as density functional theory-based methods, Monte Carlo, molecular and lattice dynamics simulations, tight-binding and effective medium approaches, order-N methods, mixed-basis methods, quasi-continuum

approaches, quantum Monte Carlo, genetic algorithm, etc and their applications to different materials.

The Conference program will include Plenary Lectures, Invited Lectures, and Poster Presentations. A few short presentations will be selected from contributions to highlight hot topics and new developments.

PROVISIONAL LIST OF INVITED SPEAKERS

O. K. Andersen

Max-Planck Institute for Festkorperforschung, Heisenberg Strasse
Stuttgart, Germany

N. Allan

School of Chemistry, University of Bristol,
Bristol, U K

V. R. Belosludov

Nikolaev Institute of Inorganic Chemistry, RAS (Sib. div.)
Novosibirsk, Russia

G. P. Das

TPPED, Bhabha Atomic Research Centre,
Mumbai, India

I. Dasgupta

Department of Physics and Metereology, Indian Institute of Technology Kharagpur,
Kharagpur, India

J. Dong,

Nanjing University, Nanjing,
China

Y. P. Feng,

National University of Singapore,
Singapore

J. Ihm,

Seoul National University,
Seoul, South Korea

T. Ikeshoji

Research Institute for Computational Sciences (RICS)
National Institute of Advanced Industrial Science and Technology (AIST),
Tsukuba, Japan

D. G. Kanhere

University of Pune, Physics Department, Ganeshkhind Pune,
India

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

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

M. Kohyama,
Interface Science Research Group,
Special Division for Green Life Technology,
National Institute of Advanced Industrial Science and Technology,
Osaka, Japan

V. I. Kosyakov
Nikolaev Institute of Inorganic Chemistry, RAS (Sib. div.),
Novosibirsk, Russia

V. Kumar
Institute for Materials Research, Tohoku University, Sendai, Japan & VKF, Chennai, India

F. A. Kuznetsov
Nikolaev Institute of Inorganic Chemistry, RAS (Sib. div.),
Novosibirsk, Russia

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

E. G. Maksimov
PN Lebedev Physical Institute, Russian Academy of Sciences,
Moscow, Russia

M. Mikami
Research Institute for Computational Sciences (RICS)
National Institute of Advanced Industrial Science and Technology (AIST)
Tsukuba, JAPAN

A. Mookerjee
S.N. Bose National Centre for Basic Sciences, Salt Lake City
Kolkata, India

I. V. Murin
St.Petersburg State University,
St.Petersburg, Russia

D. Nguyen-Manh
Theory and Modelling Department, UKAEA,

Culham Science Centre, Abingdon,
Oxfordshire, UK

R. B. Tao
Department of Physics, Fudan University, Shanghai, China

K. Ohno
Department of Physics, Yokohama National University
Yokohama, Japan

M. R. Philpott
National University of Singapore, Department of Materials Science,
Singapore

A. Postnikov
Institute of Metal Physics, Russian Academy of Sciences
Yekaterinburg 620219, Russia, &
Osnabrueck University - Department of Physics
Osnabrueck, Germany

Z. Shi
Fudan University, Shanghai
China

V. M. Tapilin
Boreskov Institute of Catalysis RAS (Sib. div.),
Novosibirsk, Russia

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

M. Tsukada
University of Tokyo, Department of Physics,
Tokyo, Japan

Z. Sh. Yanovitskaya,
Institute of Semiconductor Physics RAS (Sib. div.),
Novosibirsk, Russia

AIDA-KAWAZOE PRIZE

Three Aida-Kawazoe prizes will be given for best paper presented in the Conference to encourage young researchers.

PUBLICATION OF THE PROCEEDINGS

The proceedings of the Conference will be published. Participants should bring the manuscripts at the time of the Conference, which will be refereed. Instructions for preparation of manuscripts will be sent in due course of time.

INTERNATIONAL ADVISORY COMMITTEE

M. Ahmed, University of Dhaka
O. K. Andersen, Max-Plank Institute, Stuttgart
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G. P. Das, BARC
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K. Esfarjani, Sharif Institute of Technology
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P. Jena, Virginia Commonwealth University
Y. Kawazoe, Tohoku University
V. Kumar, Tohoku University/Vijay Kumar Foundation
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R. B. Tao, Fudan University
K. Terakura, AIST, Tsukuba
M. Tsukada, University of Tokyo
L. T. Wille Florida Atlantic University

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V. E. Panin, Institute of Strength Physics and Material sciences, SB RAS
I. V. Murin, St.Petersburg State University
I. G. Neizvestnii, Institute of Semiconductor Physics, SB RAS
G. M. Zhidomirov, Boreskov Institute of Catalysis, SB RAS

LOCAL ORGANIZING COMMITTEE

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V. R. Belosludov – Convener
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CORRESPONDENCE ADDRESS

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CONFERENCE FEE

For participants from abroad: US\$150
For participants from Russia: Rub. 500
For students from Russia: Rub. 200
(Rates for Russian delegates have been subsidized with the funding from the government of Russia)

The conference fee will cover arrival and departure transportation from the airport to the hotel, welcome reception, registration, book of abstracts, coffee breaks, refreshments, banquet and excursions but excludes accommodation charge.

The conference fee (in US dollars or an equivalent amount of EURO) should be transferred to the account of «**Institute of Inorganic Chemistry, ACCMS-2**» as is shown below:
(Payment by cheque is not acceptable)

For payment in EURO:

Intermediary Bank: OST-WEST HANDELSBANK AG
FRANKFURT/MAIN GERMANY
SWIFT: OWHBDEFF
Account: # 0104108394
Beneficiary Bank: SIBACADEMBANK
16, Prospect Lavrentieva Novosibirsk,
630090, Russia
SWIFT: SIBMRU55
Beneficiary: Institute of Inorganic Chemistry
Account: # 40503978900201000005

For payment in USD:

Intermediary Bank: Union Bank of California International New York
SWIFT: BOFCUS33NYK
ABA: 026005050

CHIPS: 0505
Account: # 91-282004-1121
Beneficiary Bank: SIBACADEMBANK
16, Prospect Lavrentieva, Novosibirsk, 630090, Russia
SWIFT: SIBMRU55
Beneficiary: Institute of Inorganic Chemistry
Account: # 40503840300201000005

In case an invoice for the payment of the conference fee through the Bank is needed, it will be sent to you on request.

The deadline for the receipt of the conference fee is June 1, 2004.

FINANCIAL SUPPORT

Partial support may be offered on request, to a limited number of young participants below the age of 35 years.

ABSTRACTS

Abstracts should be submitted through **e-mail** at the addresses bel@casper.che.nsk.su and talgat@imr.edu as **attached RTF files**, in the following format:

All abstracts must fit into one A4 page (including figures and references), aligned in width, using 11 point font and type Times New Roman, one and half spacing, 2.0 cm left and right margins, 2.0 cm spacing from the top and 4.0 cm spacing from the bottom of the sheet.

Please, provide on the top of the page: **title (capital letters)**; next line, the **names** of all **authors** (small letters, name of speaker should be marked with *); next line, the **affiliation** (institute and address, made in italic type).

The deadline for receipt of abstracts is April 1, 2004.

ACCOMODATION

Participants will be accommodated at the Hotel «Golden Valley», which offers good and inexpensive accommodation. The hotel is located at walking distance from the conference center (5-10 min.).



In order to book the hotel, please complete the **accommodation form** and send it to the Secretariat at the e-mail address: subbot@casper.che.nsk.su. Early arrivals and late departures are accepted.

Cash payment for lodging is made at the hotel in rubles. The current rate is approximately 28.0 Rubles to 1 USD.

Accommodation form

Mr. 1

Ms. 1

Family name:.....

Given name.....

Mailing address:.....

Postal code and city:.....

Country:.....

Telephone:.....Fax:.....

E-mail:.....

Arrival date.....Flight No:.....Time.....

Departure date.....Flight No:.....Time.....

- Single room (ca. 45\$ per night)
- Double room apartment (ca. 60\$ per night)
- Twin-bedded room (ca. 50\$ per night) / (ca. 25\$ per person)

For more details see: www.gold-valley.academ.org

Deadline for receipt of the accommodation form is June 15, 2004.

TRANSPORTATION

Novosibirsk is easily accessible by plane. The information can be obtained from the web site <http://english.s7.ru/> and <http://www.aeroflot.ru/eng/>. Direct flights from Frankfurt, Hannover, Seoul are made by «Siberia» airlines (S7).



Useful travel information can be received from the website www.travelocity.com or by e-mail: memberservice@travelocity.com

The Organizing Committee will provide bus transportation from the airport to the hotel. Details will be e-mailed to the participants later according to the declared arrival and departure schedule.

VISA

Visa is necessary for a visit to Russia. The rules for making visa application are rather complicated and participants are advised to apply well in advance. A personal invitation will

be sent to any scientist requiring one in order to obtain a visa to attend the meeting. To facilitate and make visa in time, please give us the following information:

1. Dates of visit
2. Full name
3. Position
4. Organization, address of organization, fax number
5. Place of birth (city, country)
6. Home address (city, country)
7. City, where you plan to get visa
8. Route
9. Full mailing address
10. Copy of the first page of your passport (jpg or pdf format)

The above information should be sent by e-mail to the Secretary of ACCMS-2, Ksenya Syrtseva to the address: ksevias@che.nsk.su **before April 1, 2004 for arranging visa invitation letter.**

Further information concerning scientific program of the Conference, excursions, etc. will be available on our website: (<http://www-lab.imr.edu/~accms/>) and on the website of Nikolaev Institute of Inorganic Chemistry SB RAS (http://www.che.nsk.su/events_en/).

IMPORTANT DATES:

April 1, 2004 _____ **Deadline for receipt of abstracts**

April 1, 2004 _____ **Deadline for submitting necessary information for arranging visa invitation letter**

June 1, 2004 _____ **Deadline for receipt of conference fee**

June 15, 2004 _____ **Deadline for receipt of the accommodation form**