

Proposal for a Psi-k workshop:

Towards reality in nanoscale materials

Abstract

The aim of the proposed workshop is to bring together representatives of solid-state physics and materials science communities who use theoretical computational tools to present and discuss state-of-the-art developments and perspectives of solid-state, computational and molecular physics techniques in modeling of non-ideal nanoscale materials. In addition to theoretical advances, progress in experiments will be covered by several invited speakers who are experts in the relevant experimental areas.

Organizers:

Dr. Adam Foster,
Laboratory of Physics, Helsinki University of Technology,
P.O. Box 1100, FIN 02015, Finland
Tel: +358-9-451 3103
Fax: +358-9-451 3116
asf@fyslab.hut.fi

Dr. Arkady Krasheninnikov,
Accelerator Laboratory, University of Helsinki,
P.O.Box 43 (Pietari Kalmin katu 2), FIN 00014
FINLAND
tel. +358-9-19150010
fax +358-9-19150042
akrashen@acclab.helsinki.fi

Prof. Risto Nieminen
Laboratory of Physics, Helsinki University of Technology,
P.O. Box 1100, FIN 02015, Finland
Tel: +358-9-451 3105
Fax: +358-9-451 3116
rni@fyslab.hut.fi

Organized as part of the Psi-k Programme, working group 7: Semiconductors and Nanotechnology

Dates and Venue:

Early December 2007, Lapland, Finland

Scientific Summary

As the scale of materials science approaches the nano, deviations from ideality become increasingly important, and standard assumptions on the role of defects and impurities on materials properties are rarely valid. For example, even a single point defect changes significantly the tensile strength and conductance of carbon nanotubes, as they are essentially one-dimensional objects. Defects are often dominant in chemical reactions, acting as key sites for molecular and cluster adsorption, even enhancing the reactivity of catalysts. In this workshop we aim to bring together experts in studying

these *deviations* from the ideal, whose work has demonstrated the importance of building a model system as close to reality as possible. The main topics of the workshop are as follows:

- **Methods** - application of first principles methods to atomistic modeling of non-ideal nanoscale materials. Including advanced approaches for studying excited states and very large systems.
- **Multiscale** – approaches to link first principles calculations to larger scale methods, such as kinetic Monte Carlo.
- **Defects in nano-structured carbon materials** – including the study of how mechanical and electronic properties of nano-structured carbon materials are influenced by defects.
- **Surface chemistry at the nanoscale** – particular emphasis will be placed on those systems where defects and impurities clearly dominate reactive properties.
- **Defect creation** – studies of doped and irradiated nanoscale materials.
- **Defect control** – beyond just studying and understanding the properties of defects and impurities, we wish to explore avenues of atomic scale control: charging; optical excitation; mechanical manipulation. This direction leads to the possibility of tailoring the electronic structure of nanoscale systems.

The results obtained for a particular system can often be transferred to another one, or generalized for a class of materials. In a similar way, methods of defect simulations developed for a system can be applied to new objects.

Workshop Programme

Day	1	2	3
9:00 – 10:30	Presentations	Presentations	Presentations
10:30 – 11:00	Coffee	Coffee	Coffee
11:00 – 12:30	Presentations	Presentations	Presentations
12:30 – 14:00	Lunch	Lunch	Lunch
14:00 – 15:30	Presentations	Presentations	Presentations
15:30 – 17:00	Posters/Refreshments	Posters/Refreshments	Posters/Refreshments
17:00 -	Free	Dinner	Free

Poster presenters will be given the opportunity to briefly introduce their posters on the first afternoon, and then posters will be available throughout the conference.

Budget

Outgoing

Expenditure	Cost (€)	Total (€)
Accommodation	40 x 400	16 000
Meals and refreshments	40 x 100	4 000
Travel	20 x 500	10 000
Local infrastructure	1 x 2000	2000
Total		32 000

Incoming

Income source	Value (€)	Status of the application
Academy of Finland	11 000	approved
Finnish National Graduate School in Materials Science	10 000	pending
National Foundations	1300	to be submitted
Psi-k network	9 700	this application
Total	32 000	

We expect about 40 people to attend the workshop, with at least half that being students and junior post. docs. Hence, for a three-day workshop, we anticipate that accommodation and food costs for each participant will be about 500 €, for a total of 20 000 €. We would further like to subsidize the travel costs of invited speakers, students and participants of limited resources at an estimated cost of 10 000 € (20 x 500 €). Minor costs related to local infrastructure e.g. room hire, proceedings etc. will total about 2000 €. We have already acquired 11 000 € funding via the academy of Finland for the workshop, and will apply for a further 10 000 € from the Finnish National Graduate school in Materials Science, and 1300 € from a Finnish National Foundation. The remaining 9700 € we ask from the Psi-k network.

Provisional list of speakers

Experiment

Philip Collins, Columbia University, USA - Identifying point defects in low-dimensional systems

Florian Banhart, University of Mainz, Germany - Engineering carbon nanostructures by electron irradiation

Jeppe Lauritsen, iNano, Aarhus University, Denmark – SPM studies of reactivity at the atomic scale

Claude Henry/Clemens Barth, CNRS Marseille, France – High-resolution AFM studies of metal clusters on insulators

Renald Schaub, St. Andrews University, Scotland - Defect chemistry on oxide surfaces

Jascha Repp, IBM Zurich, Switzerland – Controlling charging and bonding at the atomic scale

Melissa Hines - Cornell University, USA - Using chemistry to control surface morphology

Theory

Michael Moseler, University of Freiburg, Germany - Simulations of surface evolution under irradiation

Alexander Shluger/Peter Sushko, University College London, UK – Simulations of excited defect states in insulating surfaces

Hannu Hakkinen, Jyväskylä University, Finland – Modelling metallic nanoclusters

Stefano Fabris - INFM-CNR DEMOCRITOS National Simulation Center, Trieste, Italy – Simulating defect chemistry on oxide surfaces

Lev Kantorovich, King's College London, UK – Manipulation of defects and molecules at surfaces

Angelos Michaelides, Fritz-Haber Institut der Max Planck Gesellschaft, Berlin, Germany – Water chemistry on surfaces

Kai Nordlund, University of Helsinki, Finland - Multi-scale modeling of defects in low-dimensional systems

Miguel Marques, Departamento de Física Universidade de Coimbra, Portugal – Applications of Time-Dependent Density Functional Theory

Werner Hofer, Liverpool University, UK – STM studies of surface defects

Peter Haynes, University of Cambridge, UK – Linear scaling approaches to materials challenges

Miguel Gosálvez, Nagoya University, Japan – Multiscale modelling of wet chemical etching

David Tomanek, Michigan State University, USA – Simulations of defected and pristine carbon nanotubes

Curriculum Vitae

Adam Stuart Foster PhD MPhys MInstP

Date and place of birth: 4th April 1975, Birmingham, England

Gender: Male

Address: Laboratory of Physics
Helsinki University of Technology
PO Box 1100
02015 Finland

Email: asf@fyslab.hut.fi

Web: www.fyslab.hut.fi/~asf

Academic career

Period	Institution	Position
8/2004 -	Laboratory of Physics, Helsinki University of Technology	Academy of Finland senior research fellow
9/2000 -7/2004	Laboratory of Physics, Helsinki University of Technology	Postdoctoral researcher
9/1997 - 9/2000	Department of Physics and Astronomy, University College London	Postgraduate researcher
9/1996 - 5/1997	Department of Physics, Newcastle University	Research assistant - master's project Theory of the inhomogeneous electron gas
6/1996 - 9/1996	Department of Physics, Newcastle University	Research assistant - summer project Atomic scattering in ion traps

Awards

- March 1999, Interdisciplinary Surface Science Conference 12 Chester College, UK, Non-contact Atomic Force Microscopy Theoretical Imaging of Islands on the NaCl(001) Surface - awarded prize for outstanding student presentation.
- Elected to Member of the Institute of Physics, UK (2002).
- Awarded Academy of Finland senior Fellowship (8/2004 - 1/2010).

Other academic and professional activities

- Leader of Surface and Interfaces at the Nanoscale (SIN) group - www.fyslab.hut.fi/~asf/physics
- Referee for Surface Science (1999 -), Applied Surface Science (1999 -), Applied Physics A (2000 -), Physical Review B (2003 -), Nanotechnology (2003 -), and Physical Review Letters (2004 -).
- Author of textbook - Scanning Probe Microscopes : Atomic scale engineering by forces and currents' Adam S. Foster and Werner A. Hofer Springer, New York (2006)
- Supervised 4 Phd students and 8 undergraduate researchers
- Published over 50 refereed articles and 6 reviews.

Phd Defense: London, UK, November 22, 2000

Career breaks: Parental leave 10/12/05 – 27/3/06 granted by the Academy of Finland

Five most relevant publications (2001-2006):

1. Vacancy and interstitial defects in hafnia - A. S. Foster, F. Lopez Gejo, A. L. Shluger and R. M. Nieminen *Physical Review B* 65 (2002) 174117
2. Mechanism of interstitial oxygen diffusion in hafnia - A. S. Foster, A. L. Shluger and R. M. Nieminen *Physical Review Letters* 89 (2002) 225901
3. Simulating atomic force microscopy imaging of the ideal and defected TiO₂ (110) surface - A. S. Foster, O. H. Pakarinen, J. M. Airaksinen, J. D. Gale and R. M. Nieminen *Physical Review B* 68 (2003) 195410
4. Chemical identification of point defects and adsorbates on a metal oxide surface by atomic force microscopy - Jeppe V. Lauritsen, Adam S. Foster, Georg H. Olesen, Mona C. Christensen, Angelika Kühnle, Stig Helveg, Jens R. Rostrup-Nielsen, Bjerne S. Clausen, Michael Reichling and Flemming Besenbacher *Nanotechnology* 17 (2006) 3436
5. High resolution scanning force microscopy of gold nanoclusters on the KBr (001) surface - O. H. Pakarinen, C. Barth, A. S. Foster, R. M. Nieminen and C. R. Henry *Phys. Rev. B* 73 (2006) 235428

Curriculum Vitae

11.09.2006

Arkady V. Krasheninnikov, Ph.D. (Physics), Docent

ADDRESS (1): Accelerator Laboratory, University of Helsinki, P.O.Box 43
(Pietari Kalmin katu 2), FIN 00014, FINLAND TEL: +358-9-19150010

FAX: +358-9-19150042

ADDRESS (2): Laboratory of Physics, Helsinki University of Technology,
P.O. Box 1100, FIN 02015, Finland TEL: +358-9-4513138 FAX: +358-9-
4513116

E-MAIL: akrashen@acclab.helsinki.fi, ark@fyslab.hut.fi

WWW: <http://www.acclab.helsinki.fi/~akrashen/>

EDUCATION AND ACADEMIC DEGREES

Docent degree from University of Helsinki, 2005.

Ph.D. Degree in Physics (Solid State Physics), Moscow State Engineering Physics Institute, 1995.
Thesis "The effect of defects and nonmagnetic impurities on the superconducting correlations with *s*- and *d*- symmetry in high-temperature superconductors".

Master Degree (with Special Honor) in Physics (Solid State Physics), Moscow State Engineering Physics Institute, 1992. Thesis: "Computer simulation of high temperature superconductors within the framework of extended Hubbard model by quantum Monte-Carlo and exact diagonalization methods".

CURRENT POSITION

Senior scientist, Accelerator Laboratory, University of Helsinki.

and

Researcher, Laboratory of Physics, Helsinki University of Technology

PREVIOUS POSITIONS

Sep 2005 – Jul 2006 Academy Fellow, Accelerator Laboratory, University of Helsinki.

Jan 2005 – Aug 2005 Researcher, Laboratory of Physics, Helsinki University of Technology

Mar 2001-Dec 2004, Researcher, Accelerator Laboratory, University of Helsinki.

Feb 1999-Feb 2001, Associate Professor, Department of Superconductivity and Nanostructures, Moscow State Engineering Physics Institute.

May 1995-Feb 1999 Researcher, Moscow State Engineering Physics Institute.

May 1992- May 1995 Post-graduate student, Moscow State Engineering Physics Institute.

RESEARCH EXPERIENCE

15 years of experience in various topics of computational and solid state physics:

Computer simulations in irradiation effects in solids;
Electronic structure calculations at the DFT and tight-binding levels of theory;
Empirical-potential atomistic simulations;
Effects of ion irradiation on carbon nanostructures;
Simulation of scanning tunneling microscopy (STM) images; theory of STM;
Theoretical investigation of semiconductor nanosystems, including resonant-tunneling structures, quantum-cascade lasers and nano-scale quantum devices for nanocomputing;
Quantum computing in solid-state systems;
Theoretical study and computer modeling of the influence of radiation defects and impurities on both normal and superconducting properties of superconductors;
Strongly correlated systems; exact diagonalization of finite clusters.

AREAS OF INTEREST

Electronic structure calculations
Carbon nanotubes and other carbon systems;
Irradiation effects in solids;
Theory of STM;
Electronic transport in nanosystems (quantum cascade lasers, resonant-tunneling structures);
Influence of defects and impurities on electronic properties of solids;
Mechanisms of superconductivity in high-temperature superconductors;
Quantum computing in solid-state systems.

PUBLICATIONS

65 publications (only refereed papers counted).

INVITED TALKS AT INTERNATIONAL CONFERENCES

"Ion irradiation of carbon nanotubes and related phenomena", EMRS Spring Meeting, Strasbourg, France (2003); http://www-emrs.strasbourg.fr/2003SPRING/2003ABSTRACTS/2003_E_ABS.PDF

"Irradiation effects in carbon nanotubes", Nanotec03, Brighton, UK (2003) [selected from contributed]; <http://www.hpc.susx.ac.uk/nanotec/>

"Ion irradiation of carbon nanotubes", International Workshop on Interactions Between Nanostructures and Particle Beams, Shanghai, China, March 2004, <http://iwinp.sinr.ac.cn>

"Ion irradiation as a tool to tailor properties of carbon nanotubes", CAMELELENA workshop, Helsinki, Finland, September 2004, <http://www.acclab.helsinki.fi/nanotubes/meeting.html>

"Ion irradiation of carbon nanotubes", Nanotubes and nanostructures, Frascati, Italy, October 2004, <http://www.lnf.infn.it/conference/nn2004/>

"Irradiation effects in carbon systems", Advances in Functional Materials, Maroochydore, Australia, 30 Nov-02 Dec 2005.

"Irradiation of Carbon Nanotubes: Theoretical Predictions and Experimental Results", 8th international conferences on Computer Simulation of Radiation Effects in Solids, Richland, USA, June 2006, <http://cosires2006.pnl.gov>

PERSONAL AWARDS

1993-1995 Individual grant and Certificate of Qualification from the Humantech Scholarship, **Samsung Electronics Corporation (South Korea)**.
1994-1995 Individual post-graduate grant No A44-F from the **International George Soros Science Foundation (ISSEP)**.
1997-2000 Individual grant from the **Russian Academy Of Sciences "Young Scientists of Russia"**.
2001 Travel grants from the **Magnus Ehrnrooths Foundation (Finland)**.
2002 Travel grants from the **Magnus Ehrnrooths Foundation (Finland)**.
2003 Travel grants from the **VŠisŠIŠ Foundation (Finland)**.
2004 Travel grants from the **Magnus Ehrnrooths Foundation (Finland)**.
2005 Travel grants from the VŠisŠIŠ Foundation (Finland).
2005 Academy Fellow (temporary) position, Academy of Finland
2006 Research/travel grant from Academy of Finland and DAAD (Deutscher Akademischer Austauschdienst), project leaders Docent A. Krasheninnikov (Finland) and Professor F. Banhart (Germany).

WORK UNDER SCIENTIFIC CONTRACTS

1996-97 Contract DSWA01-97-C-0050 "Energy and Kinetics of Phase Transitions in Solids with High Concentration of Point-Defect" from **Defense Agency Of Special Weapons (USA)**.
1997-98 Contract DSWA01-97-C-0055 "Physical Aspects of Energy Accumulation and Release in Small Particles and Nanostructures" from **Defense Agency Of Special Weapons (USA)**.
1999-00 Contract DSWA01-99-M-0523 "Energy Accumulation and Release in Highly Non-equilibrium Ensembles of Small clusters" from **Defense Threat Reduction Agency (USA)**.

CONFERENCE ORGANIZATION:

International workshop on physics and chemistry of carbon nanotubes "ELENA-CAMEL meeting", 2004, Helsinki, Co-chairman,
<http://www.acclab.helsinki.fi/nanotubes/meeting.html>

REFEREE FOR THE JOURNALS AND PROJECT EVALUATION:

Phys. Rev. Lett., Phys. Rev. B, Nanoletters, Carbon, Physica E, Materials Science and Engineering B, Physics of Low-Dimensional Structures, Scripta Materialia.

Evaluators of projects submitted to Irish Science Foundation (Ireland), Petroleum Research Fund (USA).

OTHER ADMINISTRATIVE DUTIES:

Member of the Editorial Board of Computational and Theoretical Nanoscience

TEACHING EXPERIENCE AND GRADUATE SUPERVISION

"Materials Physics II", Helsinki University of Technology, 2005, lectures.
<http://www.fyslab.hut.fi/kurssit/Tfy-3.461/>

"Introduction to electronic structure calculations", University of Helsinki, 2002 (<http://www.acclab.helsinki.fi/~akrashen/esctmp.html>), lectures and exercises.
"Theoretical superconductivity", Moscow State Engineering Physics Institute, 1999-2000, lectures and exercises.
"Computational Physics"; Moscow State Engineering Physics Institute, 1998-2000, lectures and exercises.
"Physics of phase transitions", Moscow State Engineering Physics Institute, 1999, exercises.

Supervised/co-supervised works of Ph.D. 4 students and 7 M. Sc. students.

SCIENTIFIC VISITS/SEMINARS

Feb 1991, Basel Solid - State Physics Institute, Basel University, Basel, Switzerland.
Jan 2000, Laboratory of Physics, Helsinki University of Technology, Finland.
Jun 2000, Georg-August Universitaet, II Physicalisches Institut, Goettingen, Germany
Oct 2000, Institut für Theoretische Physik, Technische Universität Berlin, Germany.
Feb 2002, Weizmann Institute of Science, Rehovot, Israel
Jun 2003, Forschungszentrum Rossendorf, Dresden, Germany.
Feb 2004, Virtual Materials Laboratory, Delft, the Netherlands.
Jun 2004, University of Darmstadt, Darmstadt, Germany.
Nov 2004, University of Oxford, UK.
Nov 2005, University of Dublin, Ireland.
Apr 2006, University of Mainz, Germany.

PERSONAL DATA

Date and place of birth: December 13, 1967, Moscow, Russia
Sex: Male
Citizenship: Russian
Marital status: Married; Children: 1 child (born May 2005)
Languages: Russian (native), English (fluent), German (mediocre).
Military service: 1986-1988 (two full years), military rank - sergeant.

Selected publications

1. L. Sun, F. Banhart, **A.V. Krasheninnikov**, J.A. Rodriguez-Manzo, M. Terrones and P.M. Ajayan, "Carbon nanotubes as high-pressure cylinders and nano-extruders", *Science* 312 (2006) 1199.
2. J. A. Åström, **A. V. Krasheninnikov**, and K. Nordlund, "Carbon nanotube mats and fibers with irradiation-improved mechanical characteristics: a theoretical model", *Phys. Rev. Lett.* 93 (2004) 215503.
3. P.O. Lehtinen, A.S. Foster, Y. Ma, **A.V. Krasheninnikov**, and R. M. Nieminen "Irradiation-induced magnetism in graphite: a density-functional study", *Phys. Rev. Lett.* 93 (2004) 187202.
4. P.O. Lehtinen, A.S. Foster, A. Ayuela, **A.V. Krasheninnikov**, K. Nordlund, and R. M. Nieminen, "Magnetic properties and diffusion of adatoms on a graphene sheet", *Phys. Rev. Lett.* 91 (2003) 017202.
5. **A.V. Krasheninnikov**, K. Nordlund, M. Sirviö, E. Salonen and J. Keinonen "Formation of ion irradiation-induced atomic-scale defects on walls of carbon nanotubes", *Phys. Rev. B* 63 (2001) 245405.

Prof. Risto M. Nieminen - short CV

(for a full CV, see http://www.fyslab.hut.fi/home/Risto_Nieminen.html)

b. 1948 Helsinki, Finland
Dr.Sc. (Tech.) 1975 Helsinki University of Technology

Academic career

Research Fellow, Cambridge University, 1973-5

Research Fellow, NORDITA, Copenhagen, Denmark , 1975-7

Associate Professor, University of Jyväskylä, Finland, 1978-1986

Visiting Professor, Cornell University, USA, 1979-80, 1986-7

Professor of Physics, Helsinki University of Technology, 1987-present
Scientific Director, Center for Scientific Computing, 1989-1996

Academy Professor, 1997 – 2002, 2003-

Leader of the COMP unit at Helsinki University of Technology with 60 researchers. COMP has been designated as a National Center of Excellence in Research by the Academy of Finland.

Research areas

Theoretical and computational condensed-matter and materials physics; nanosciences and nanotechnology; high-performance computing.

Publication activity

352 refereed original and 51 refereed review publications in condensed matter and materials physics journals, books and monographs. These articles have received more than 8000 citations in the SCI database. More than 120 other articles, including conference proceedings, numerous popular articles and media presentations.

Graduate and post-doctoral supervision

Supervised 35 Ph.Ds during 1978-2004. Chairman of the National Graduate School in Materials Physics since 1994. Board member in the Swedish National Graduate School in Scientific Computing since 1999.

Supervised 22 post-doctoral fellows during 1981-2002.

Conference activities

123 invited and plenary talks at international conferences. Member of the organisation committees of 80 international conferences.

Current scientific editorships

Editor, Computational Materials Science (Elsevier); Lecture Notes in Computational Science and Engineering (Springer); Physica Scripta; Materials Science Forum; Journal of Scientific Programming; Journal of Computational Methods in Science and Engineering; Journal of Computational and Theoretical Nanoscience.

Recent international scientific duties

Member of the CERN Council and Committee of Council, 1996-2002.

Member and chairman of the NORDITA (Copenhagen) Board, 1990-1996, and its Condensed Matter Committee, 1996-2002.

Member of the IUPAP Commission on Computational Physics since 1996 (secretary 1999-2002, vice-chairman 2003-).

Member, Management Committee, COST Program on Simulation of Physical Phenomena in Technological Applications, 1997-2001 .

Member, Management Board, EU Training and Mobility of Researchers Network on Electronic Structure Calculations of Materials Properties and Processes for Industry and Basic Research, 1998-2003.

Member, Steering Committee, European Science Foundation (ESF) Programme on Electronic Structure Calculations Elucidating the Complex Atomistic Behaviour of Solids and Surfaces, 1998-2002.

Member, Steering Committee, European Science Foundation (ESF) Programme on Electronic Structure Calculations Elucidating the Complex Atomistic Behaviour of Solids and Surfaces, 2003 - .

Member, International Advisory Board, Center for Computational Materials Science, University of Vienna, Austria, 1999- .

Member, International Committee for Atomic Collisions in Solids (ICACS), 1999- 2004.

Member, International Advisory Committee on Positron Annihilation, 2000- 2004.

Member, International Scientific Committee for Materials Research, Spanish Scientific Research Council (CSIC), 2001- .

Member, Scientific Advisory Board, the NANOMAT Programme, Norwegian Research Council, 2003-.

Member, Scientific Advisory Board, Fritz-Haber-Institut of the Max-Planck-Society, Germany, 2004- .

Member, Scientific Advisory Board of the Helmholtz Association, Germany, 2004-.

Recent refereeing and evaluation duties

Expert evaluation of the Materials Research Consortia proposals, Stiftelsen för Strategisk Forskning, Sweden, 1999-2000 (chairman of the evaluation panel), 2002-2003

Expert evaluation of the proposals for Future Scientific Leaders, Stiftelsen för Strategisk Forskning, Sweden, 2000-2001.

Evaluation of the GROWTH Programme proposals, EU Research Directorate, 2000.

Evaluation of the Estonian Centers of Excellence in Research, 2001.

Evaluation of the Danish Initiatives in Advanced Scientific Computing, 2001.

Expert evaluation of the Materials Research Consortia proposals, Stiftelsen för Stragegisk Forskning, Sweden 2002-2003.

Evaluation of the NANOPHASE RTN, European Commission, 2002.

Member of the Evaluation Panels and Rapporteur, EU VI Framework Program, 2003- .

Member, Evaluation Panel of the Research Programmes of the Helmholtz Association, Germany, 2003-.

Evaluation of the Senior Individual Grants, Stiftelsen för Strategisk Forskning, Sweden, 2003-2004.

Evaluation of the Danish Center for Scientific Computing (DCSC), Denmark 2004.

Evaluation of the Center of Excellence Programme (Starka forskningsmiljöer), Swedish Research Council 2004.

Evaluation Panel of NORDITA, Denmark 2004 (Academic secretary of the Panel).

Journal refereeing

Article refereeing for Physical Review A, B, E; Physical Review Letters; Journal of Physics A: Mathematical and General; Journal of Physics B: Atomic and Molecular Physics; Journal of Physics C: Solid State Physics; Journal of Physics F: Metal Physics; Journal of Physics CM: Condensed Matter; Applied Physics; Solid State Communications; Physica Scripta; Physics Letters; International Journal of Quantum Chemistry; Reviews of Modern Physics; Surface Science; Chemical Physics; Journal of Chemical Physics; Chemical Physics Letters; Solid State Electronics; Semiconductor Science and Technology; Computational Materials Science; Journal de Physique; Proceedings of the Royal Society; Journal of Applied Physics; Faraday Transactions; Europhysics Letters; Journal of Measurement Science and Technology; Vacuum; Journal of Non-Crystalline Solids; Applied Physics Letters; Physica; Journal of Materials Chemistry; Journal of Vacuum Science and Technology; Nanotechnology; Physica Status Solidi; Optics Communications; Journal of Electrochemical Society, Nuclear Instruments and Methods B; European Journal of Physics B; Physical Chemistry- Chemical Physics; Nuclear Instruments and Methods B; Acta Materialia.

Research proposals

Proposal refereeing for the U.S. National Science Foundation; Research Corporation; Science and Engineering Research Council of Canada; NATO Scientific Affairs Division; EC Science Program; Flemish Regional Government (Belgium); Naturvetenskapliga Forskningsrådet (Sweden); International Science Foundation (New York, USA); Israel Science Foundation; F.O.M. (The Netherlands); Tekniskvetenskapliga Forskningsrådet (Sweden); Stiftelsen för strategisk grundforskning (Sweden); Academy of Finland; Foundation for Research Development (South Africa); Austrian Science Fund FWF (Austria); Council of Scientific and Industrial Research (India); Istituto Nazionale per la Fisica della Materia INFN (Italy); Humboldt Foundation (Germany); Physics and Astronomy Research Council (United Kingdom); European Science Foundation; Chilean Research Council; Nordisk Forskarakademi (NorFA); Deutsche Forschungsgemeinschaft (Germany); The Third World Network of Scientific Organisations; Netherlands Organisation for Scientific Research (NWO); Deutsche Forschungsgemeinschaft; Swiss National Science Foundation.

Faculty positions

Expert evaluation of candidates for professorships and lectureships : Cornell University (USA), Linköping University (Sweden, three positions), Umeå University (Sweden), Chalmers University of Technology (Sweden, four positions), NORDITA (Denmark), Uppsala University (Sweden), Technical University of Norway (five positions), University of Cape Town (South Africa); University of Witwaterstrand (South Africa), University of Crete (Greece); Luleå University of Technology (Sweden), Max-Planck-Institute (Germany).

Service on *appointment and tenure refereeing committees* for several foreign and domestic universities.

Other recent committee service

Information Strategy Commission for Education and Research, Ministry of Education 1994-5.
OECD Conference “Global Research Village”, Elsinore, Denmark 1996.

Information Society Forum, Finnish Government, 1996-1999
EU-Japan Co-operation Conference on Education, Science and Technology, Tokyo 1997.
Role of Science in Information Society, Geneva, Switzerland 2003.
Chairman, Tugnregnekommitteen, Norway , 2003-2004.
Steering Committee for the Nordic Data Grid Facility, 2003-
Chairman, United World Colleges Committee in Finland, 2003 - .
Chairman, National Strategy Group for Grid Infrastructure, 2005-

Other positions of trust

Member, Governing Board of the Finnish Cultural Foundation, 1994-; Executive Council, 1999- .
Member, Governing Board of Osk.Huttunen Foundation, 2000- .
Member, Information Technology Board, Helsinki University of Technology 1997- .
Member, EUROSCIENCE, 1998- .
Member, Board of Delegates, European Materials Research Society, 2002-.
Member, Science and Technology Policy Council of Finland, 2005-2008.

Invited lectureships

Honorary Visiting Fellow, University of New South Wales, Sydney, Australia 1982.
Honorary Visiting Fellow, University of Cambridge and Imperial College, Cambridge and London, UK 1990.
Honorary Visiting Fellow, Korea Advanced Institute for Science and Technology, 2001.

Ca. 150 invited lectures and seminars at numerous universities and laboratories.

Honors and prizes

Member, Finnish Academy of Sciences and Letters.
Member, Finnish Academy of Technology.
Fellow, American Physical Society.
Fellow, Institute of Physics (UK).
Magnus Ehrnrooth Physics Prize 1989.
University Publicists' Prize 2003.
Professor of the Year 2003.
Knight (First Class), Order of the White Rose of Finland.

Five most relevant publications (2001-2006):

1. T.E. M. Staab, R.M. Nieminen, M. Luysberg and Th. Frauenheim: Agglomeration of As antisites in As-rich LT-GaAs: nucleation without a critical nucleus size, *Phys.Rev. Lett.* **95**, 125502 (2005).
2. A. Ayuela, M.J. Puska, R.M. Nieminen and J.A. Alonso: Charging mechanism for the bond elongation observed in suspended chains of gold atoms , *Phys.Rev. B Rapid Comm.* **72**, 161403(R) (2005).
3. A.V. Krasheninnikov, P.O. Lehtinen, A.S. Foster and R.M. Nieminen: Bending the rules: contrasting vacancy migration in graphite and carbon nanotubes, *Chem. Phys. Lett.* **418**, 132 (2006).
4. M.G. Ganchenkova and R.M. Nieminen: Nitrogen vacancies as major point defects in GaN, *Phys.Rev. Lett.* **96**, 196402 (2006).
5. T. Lopenen, A.V. Krasheninnikov, M. Kaukonen and R.M. Nieminen: Nitrogen-doped carbon nanotubes under irradiation , *Phys. Rev. B* **74**, 073409 (2006).