European Science Foundation

Standing Committee for Physical and Engineering Sciences (PESC)

**ESF PESC EXPLORATORY WORKSHOP**

**Mott's Physics in Nanowires and Quantum Dots**

# Scientific Report

**Cambridge,**
**United Kingdom, 31 July – 2 August 2006**


**Convened by**

**Sasha Alexandrov**

Department of Physics, Loughborough University


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*Co-sponsored by*

EPSRC

Loughborough University

## 1. Executive summary

The emphasis of this workshop was on

- molecular, semiconducting and superconducting nano-objects,
- strongly correlated electrons and phonons on the nanoscale,
- low-dimensional conductors,
- metal-insulator transitions and size quantization and
- mesoscopic quantum theory including first-principle simulations.

The workshop was planned as a meeting of European researchers working in experimental nano-physics, quantum chemistry and nano-engineering and the theory of strongly correlated electrons and polarons. It helped to promote European collaboration between experimental and theoretical researchers in molecular, semiconducting and superconducting nanowires and quantum dots and strongly correlated electrons and phonons. The workshop also used the occasion to mark the centenary of the birth of Sir Nevill Francis Mott, whose research on metal-insulator transitions, polarons and amorphous semiconductors has had tremendous impact on our current understanding of strongly correlated quantum systems.

The Scientific Convenor initiated creation of the Executive Organising Commettee comprising

- Prof. Yao Liang (Cambridge University) wyl1@cam.ac.uk, Co-chairman, President of Gonville and Caius College
- Prof. Kurt Ziebeck (Loughborough University) K.R.Ziebeck@lboro.ac.uk, Co-chairman
- Dr. Jim Hague (Loughborough University) J.P.Hague@lboro.ac.uk, Treasurer
- Dr. Klaus Neumann (Loughborough University) K.U.Neumann@lboro.ac.uk
- Dr. John Samson (Loughborough University) J.H.Samson@lboro.ac.uk, Webmaster

The Commettee provided accommodation and technical assistance at the scientific sessions in Gonville and Caius College, University of Cambridge, workshop website design (http://www.lboro.ac.uk/departments/ph/nqd/index.html), workshop poster design, excursion, workshop photo, travel information, and processing of the expencies claims of participants.

The Scientific Convenor secured additional financial support from EPSRC (UK) (grant number EP/D07777X/1, university account PHJW9, 5819 Euro) and the Faculty of Science at Loughborough University (university account PHH RE, 1455 Euro), allowing for participation of a few leading researches in the field from the United States and Russia, and covering the organisation expences. Loughborough University administered these as well as the ESF grant (university account PHJ W8, 1400 Euro).

In December 2005- January 2006 invitations were sent to 31 researches actively working in the field from universities and government/corporate laboratories, and they were enthusiastically accepted by all invities. Finally two invited speakers, Prof. R. Laughlen (Stanford Universitity, US) and Prof. S. von Molnar (University of Florida, US) were unable to attend because of personal circumstances.

The participants were asked to submit their titles and abstracts well in advance, which allowed the Organising Committee to publish the Abstract book of the workshop on the website (http://www.lboro.ac.uk/departments/ph/nqd/Abstracts%20book.pdf), and distribute hard copies with the maps of Cambridge and the badges in the personal folders at the registration on Sunday, 30 July 2006. Most of the participants were accommodated at Gonville and Caius College, where all sessions, discussion meetings and meals were organised, with a few staying at Trinity and Pembroke Colleges and hotels. The lecture room was equipped with laptops and projectors for power-point and overhead presentations. Wireless internet connection was provided for those participants, who required the internet access.

The workshop was opened with the presentation of the European Science Foundation by Dr. Patrick Bressler and a special reminiscences lecture by Prof. Ted Davis (University of Cambridge), who collaborated with Sir Nevill Mott for a long time. There were 6 Panels, chaired by leading experts in the field: "Low-dimensional and nano structures" (experiment), "Polarons on nanoscale" (theory), " Polarons and bipolarons" (in bulk materials, theory), "Quantum wires and dots" (experiment and theory ), "Correlated electrons on nanoscale" (theory), and "Strongly-correlated electrons in bulk materials" (theory and experiment). The speakers had 30 minutes for their presentations and plenty of time for discussions at the discussion sessions and dinners.

The workshop ended with lunch on Wednesday, 2 August 2006, as it was planned. Travel and accommodation expences claim forms (where applicable) were distributed among the participants during the workshop, and collected and processed by Loughborough University Finance Office in August-September 2006.

Prof. Marshall Stoneham, Editor-in-Chief of the Journal of Physics: Condensed Matter (IoP) encouraged participants to publish the workshop proceedings in a special issue of this high-impact journal. JPCM is currently collecting the manuscripts, which will be published in March 2007.

## 2. Scientific contents

The integrated circuit was invented in 1959, and Jack Kilby won the Nobel Prize in Physics for this invention. Since that date, the number of transistors that can be fabricated onto a single chip has been doubling about every 18 months - an observation commonly known as Moore's Law. This exponential process has taken the world from a crude chip with a single transistor to integrated circuits with 100 million active components in only 40 years. At the same time, the amount of useful computational work that comes out of an integrated circuit for each unit of electrical power put into it has also increased by roughly 100 million. This astounding technological progress has given us what we call today the Information Age. It has had a profound effect on the lives and fortunes of people, companies and countries throughout the world. How much longer can this exponential growth continue? Ever since it was first proposed, there has been a great deal of discussion about when Moore's Law would reach a limiting plateau. There is growing belief that the progress of the silicon technology is reaching its physical, engineering and economic limits.

The fact that silicon is approaching the upper limit, however, doesn't mean that progress in computing will slow down. There are many new technologies that are being pursued in university and corporate laboratories around the world. In particular, molecular switching devices and systems that will assemble themselves through molecular recognition are being designed and investigated. Many laboratories around the world are now testing new types of reversible switches, as well as fabricating nanowires needed to connect the circuit elements together. Once one has the appropriate switches and wires, the next significant step will be integrating them together into more complex structures that perform useful functions.

There are still significant opportunities and requirements for invention and discovery on that front before molecular nanoelectronics becomes a reality. The actual mechanisms of molecular switching and transport through molecular nanowires are of the highest current experimental and theoretical value. A correlated transport through solid-state mesoscopic systems with *repulsive* electron correlations has received considerable interest in the past and continues to be the focus of intense experimental and theoretical investigations

Remarkably a number of experimental provide evidence for various molecular switching effects, where the current-voltage (I-V) characteristics show two branches with high and low current for the same voltage well below a conventional threshold in solid-state quantum dots. This phenomenon can result from a conformational transformation of certain molecules containing a "moving part" like a bypyridinium ring, which changes its position if the voltage is sufficiently high, or from the interaction of metallic leads with the molecules. These transformations necessarily involve a large displacement of many atoms so that this *ionic* switching is rather slow, perhaps operating on a millisecond scale. Switching was also observed for simple molecules self-assembled in organic molecular films. Molecular devices that exhibit intrinsic switching could be the basis of future active elements of molecular electronics. Thus further progress will depend upon finding molecules and understanding *intrinsic* mechanisms for their reversible switching from low to high current state, which could be provided by the electron-vibron interaction forming polarons ``dressed'' by phonons. The *attractive* electron correlations in bulk and nanowires could be caused by a strong electron-vibron interaction, which overscreens the Coulomb repulsion, and forms polarons instead of bare electrons. In contrast to free electrons, polarons attract each other at short distances of the order of the interatomic spacing. There are also significant opportunities for discovery of unique nanoscale phenomena arising from the dimension quantization. The onset of quantum-size effects in a finite system might signal the occurrence of a genuine metal-insulator transition on mesoscopic scale and substantially affect their conductance also in the metallic regime. *Transport properties of strongly-correlated low-dimensional conductors and molecular nanowires, polarons and bipolarons* were central topics of the workshop:

*On the experimental side* the technology of producing electrons confined to one dimensions (1D) and the role of disorder in 1D wires were discussed in the opening lecture by Mike Pepper (University of Cambridge), novel subnano structures comprising nonmetallic clusters in a metallic matrix were presented by Arndt Simon (Max-Planck-Institut, Stuttgart), exciting achievements in nano-structuring of cuprate superconductors were reviewed by Ivan Bozovic (Brookhaven) and experiments on transport in thin film constrictions with no ballistic transport were presented by Nicolás García (CSIS, Madrid) on the first day of the meeting. On the second day Tony Bland (University of Cambridge) discussed spin dynamics in ferromagnetic nanorings, functional properties and structures of inorganic molecular nanowires including magnetism were presented by Dragan Mihailović (Jožef Stefan Institute, Ljubljana), Klaus Ploog (Paul-Drude-Institut, Berlin) presented perfect quantum wires and dots with subnanometre dimensions. The Single-Atom Transistor at room temperature was presented by Thomas Schimmel (Karlsruhe University), and Peter Edwards (University of Oxford) reviewed bipolarons in metal-ammonia solutions. Carlo Taliani (ISM-CNR, Bologna) contributed to the experimental talks with a comprehensive review of organic semiconductors for spintronics.

*Theoretical talks* included extensive discussions of recent achievements in our understanding of strongly correlated electrons on nanoscale [ Alexander Andreev (Kapitza Institute, Moscow), Józef Spałek (Jagiellonian University, Kraków)), Janez Bonča (Ljubljana University), Bogdan Bułka (Institute of Molecular Physics, Poznań), Yurii Firsov (Ioffe Institute, Saint Petersburg), Holger Fehske (Ernst-Moritz-Arndt University, Greifswald)], and in bulk materials [Herbert Capellmann (RWTH, Aachen), Konstantin Efetov (Bochum University), Ferdinando Mancini (University of Salerno)]. Two panels of the meeting were devoted to polarons and bipolarons on nanoscale (Marshall Stoneham (UCL, London) , Jozef Devreese (Antwerp University), Fons Brosens (Antwerp University), Sasha Alexandrov (Loughborough University), Alex Bratkovsky (HP Labs, Palo Alto)], and in bulk inorganic and organic materials [Serge Aubry (CNRS, Saclay), Wolfgang von der Linden (University of Graz), Pavel Kornilovitch (HP Company, Corvallis)], and Martin Hohenadler (University of Graz)]. Viktor Kabanov (Jožef Stefan Institute, Ljubljana) presented novel magnetic quantum oscillations in nanowires, and Peter Littlewood (University of Cambridge) reviewed recent achievements in the Bose- Einstein condensation of exciton polaritons.

## 3. Outcomes and results

The workshop set clear directions for collaborations between experimental and theoretical European researchers of low-dimensional electronic systems, nanowires and quantum dots including their Russian and US colleagues from corporate (HP) and government (BNL, Kapitza and Ioffe Institutes) laboratories. A few initiatives for further ESF and EU meetings were discussed. 11 participants of the workshop have agreed to contribute to the book "Polarons in Advanced Materials", which is now commissioned by Canopus/ Springer Publishing with the Scientific Convenor as the editor. Proceedings of the workshop will be published in the special issue of Journal of Physics: Condensed Matter (IPO) dedicated to Sir Nevill Mott. Both Proceedings and the Book will kindly printed without charge. The workshop also marked the centenary of the birth of Sir Nevill Mott (The Nobel Prize Laureate), whose research on metal-insulator transitions, polarons and amorphous conductors has tremendous impact on our current understanding of strongly-correlated quantum systems.

The organisers received messages from many participants with their high estimate of the workshop , in particular:

"What a marvellous conference. Nevill would have loved it !" (Peter Edwards, Oxford), "The workshop was very productive for me" (Nicolas Garcia, Madrid), "The conference I found great and very enjoyable" (Jozef Devreese, Antwerp), "Congratulations on organising such

an excellent workshop and for inviting me to participate. Very well done!" (Ted Davis, Cambridge), "I enjoyed the workshop a lot and I feel I've learned much" (Bozovic, Brookhaven).

## 4. Final programme

### Sunday 30 July 2006

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| Afternoon | *Arrival, Gonville and Caius College, Cambridge* |
| 19:30 | *Welcome reception at Gonville Court (out door, weather permitting)*<br>*OR Colyton Hall (accessed by Gonville Court D Staircase)* |

### Monday 31 July 2006

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|---|---|
| 09:00 | *Welcome (Bateman Auditorium, accessed by Caius Court I Staircase)*<br>**Yao Liang** *(President, Gonville and Caius College)* |
| 09:10 | **Presentation of the European Science Foundation (ESF)**<br>**Patrick Bressler**<br>*(Standing Committee for Physical and Engineering Sciences)* |
| 09:25 | Sir Nevill Francis Mott (1905-1996) – reminiscences<br>**Ted Davis** (*University of Leicester)* |
| 09:50 | **Introduction by scientific convenor**<br>**Sasha Alexandrov** *(Loughborough University)* |

#### Panel 1: Low-dimensional and nano structures

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|---|---|
| | Chair**:** **Kurt Ziebeck** *(Loughborough University)* |
| 10:00 | Disorder and interaction effects in one dimension<br>**Mike Pepper** *(University of Cambridge)* |
| 10:25 | *Coffee break (Bateman Room)* |
| 10:55 | A glimpse into subnano structures<br>**Arndt Simon** *(Max-Planck-Institut, Stuttgart)* |
| 11:20 | Nano-structuring cuprate superconductors<br>**Ivan Bozovic** *(Brookhaven)* |
| 11:45 | Is there ballistic transport in metallic nanoobjects?<br>Ballistic versus diffusive transport<br>**Nicolás García** *(CSIS, Madrid)* |
| 12:10 | **Discussion** |
| 12: 40 | *Lunch (Senior Parlour, accessed by Gonville Court D Staircase)* |

#### Panel 2: Polarons on nanoscale

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| | Chair**:** **Peter Littlewood** *(University of Cambridge)* |
| 14:00 | Trapping and self-trapping:<br>polaronic defects in the bulk and at interfaces<br>**Marshall Stoneham** *(UCL, London)* |

14:25 Fröhlich polarons from 0D to 3D: concepts and recent developments
**Jozef Devreese** *(Antwerp University)*

14:50 Quantum statistics for a finite number of polarons in a quantum dot
**Fons Brosens** *(Antwerp University)*

15:15 Current-controlled polaronic switching of molecular quantum dots
**Sasha Alexandrov** *(Loughborough University)*

15:40 *Tea break (Bateman Room)*

### Panel 3: Polarons and bipolarons

Chair: **Marshall Stoneham** *(UCL, London)*

16:10 Ultrafast polaron transport in biosystems
**Serge Aubry** *(CNRS, Saclay)*

16:35 Magnetic polarons and phase separation in the Kondo model
**Wolfgang von der Linden** *(University of Graz)*

17:00 Monte-Carlo simulations of lattice polarons and bipolarons
**Pavel Kornilovitch** *(HP Company, Corvallis)*

17:25 Carrier-density effects in many-polaron systems
**Martin Hohenadler** *(University of Graz)*

19:30 *Dinner (Fellows' Dining Room, accessed by Gonville Court D Staircase)*

21:00 **Summary of day and after-dinner discussion**

## Tuesday 1 August 2006

### Panel 4: Quantum wires and dots

Chair**:** **Mike Pepper** *(University of Cambridge)*

08:30 Ferromagnetic nanorings
**Tony Bland** *(University of Cambridge)*

08:55 Functional properties of molecular $MoSI_x$ nanowires:
from structure to magnetism
**Dragan Mihailović** *(Jožef Stefan Institute, Ljubljana)*

09:20 Fabrication and electronic properties of perfect quantum wires and dots with subnanometre dimensions
**Klaus Ploog** *(Paul-Drude-Institut, Berlin)*

09:45 Luquid-liquid phase separation in metal-ammonia solutions.

**Peter Edwards** *(University of Oxford)*

10:10 *Coffee break (Bateman Room)*

10:40 Localisation vs delocalisation in correlated nanosystems within exact diagonalisation — ab initio approach
**Józef Spałek** (*Jagiellonian University*, *Kraków*))

11:05 Magnetic quantum oscillations in nanowires
**Viktor Kabanov** *(Jožef Stefan Institute, Ljubljana)*

11:30 The Single-Atom Transistor: An approach towards quantum electronics at room temperature
**Thomas Schimmel** *(Karlsruhe University)*

11:55 Electron transport in nanostructures, including molecular quantum dots
**Alex Bratkovsky** (*HP Labs, Palo Alto*)

12:20 *Lunch (Senior Parlour)*

### Panel 5: Correlated electrons on nanoscale

Chair**:** **Konstantin Efetov** *(Bochum University)*

14:00 Manifestation of additional dimensions of space-time in semiconductor quantum dots
**Alexander Andreev** *(Kapitza Institute, Moscow)*

14:25 Spin-charge separation in quantum nanowires: theory and experiment
**Yurii Firsov** *(Ioffe Institute, Saint Petersburg)*

14:50 Luttinger liquid, Peierls or Mott insulator: quantum phase transition in one-dimensional electron-phonon systems
**Holger Fehske** *(Ernst-Moritz-Arndt University, Greifswald)*

15:15 *Tea break (Bateman Room)*

15:45 Conductance through coupled quantum dots
**Janez Bonča** *(Ljubljana University)*

16:10 Correlated electrons and transport in nanostructures
**Bogdan Bułka** (*Institute of Molecular Physics, Poznań*)

16:35 **Summary of day, discussions and excursion**

19:30 *Conference Dinner (Fellows' Dining Room)*

## Wednesday 2 August 2006

### Panel 6: Strongly-correlated electrons in bulk materials

Chair: **Jozef Devreese** *(Antwerp University)*

09:00 Condensation of exciton polaritons
**Peter Littlewood** *(University of Cambridge)*

09:25 The interplay between superconductivity and magnetism
**Herbert Capellmann** *(RWTH, Aachen)*

09:50 *Coffee break (Bateman Room)*

10:20 Non-Fermi liquid behaviour of a Fermi gas with a repulsion
**Konstantin Efetov** *(Bochum University)*

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| 10:45 | Non-Fermi liquid behaviour and pseudogap opening in the 2D Hubbard model within COM<br>**Ferdinando Mancini** *(University of Salerno)* |
| 11:10 | Organic semiconductors for spintronics<br>**Carlo Taliani** *(ISM-CNR, Bologna)* |
| 11:35 | **Discussion of future collaborative research activities and closing remarks** |
| 13:00 | *Lunch (Senior Parlour)* |
| 14:00 | *Workshop ends* |

## 5. Statistical information on participants.

- *Age structure:* 30-40 years old (4), 40-50 years old (8), 50-60 years old (7), above 60 (11).
- *Countries of origin:* Austria (2), Belgium (2), France (1), Germany (6), Italy (2), Poland (2), Russia (2), Slovenia (3), Spain (1), United Kingdom (6), United States (3).

## 6. Final list of the participants.

1. Prof. Sasha Alexandrov, Physics Department, Loughborough University, Loughborough LE11 3TU, UK,
tel: +44 1509223303, fax: +44 1509223986, e-mail: a.s.alexandrov@lboro.ac.uk

2. Prof. Alexander Andreev, P.L. Kapitz Institute for Physical Problems, Kosygin str. 2, 119334 Moscow, Russia,
tel:+7 495 6512124, fax: +7 495 6512125, e-mail: andreev@kapitza.ras.ru

3. Dr. Serge Aubry, CEA Saclay-CNRS, 91191 Saclay, Gif-sur-Yvette Cedex, France,
e-mail: Serge.Aubry@cea.fr

4. Prof. Tony Bland, Cavendish, Cambridge University, Madingley Road, Cambridge CB3 OHE, UK,
tel: +44 1223 337436, fax: +44 1223 350266, e-mail: jacb1@phy.cam.ac.uk

5. Prof. Janez Bonca, Department of Physics, Ljubljana University, Jadranska 19, 1000 Ljubljana, Slovenia,
tel: +386 1 476 6561, fax: +386 1 251 7281, e-mail: Janez.Bonca@ijs.si

6. Dr. Ivan Bozovic, Brookhaven National Laboratory, Condensed Matter Physics and Material Science, P.O. Box 5000, Upton NY 11973-5000, US, e-mail: bozovic@bnl.gov

7. Dr. Alex Bratkovsky, Hewlett-Packard Labs, 1501 Page Mill Road, 1L, Palo Alto CA 94304, US,
tel: +1650 8577355, fax: +1650 8577179, e-mail: alex.bratkovski@hp.com

8. Dr. Patrick Bressler, European Science Foundation, 1 quai Lezay-Marnésia, BP 90015, 67080, Strasbourg Cedex, France, e-mail: pbressler@esf.org

9. Prof. Fons Brosens, Department of Physics, Antwerp University, Campus Drie Eiken G.U314, Groenenborgerlaan171, 2610 Antwerpen, Belgium,
tel: +32 653433, fax: +32 653318, e-mail: fons.brosens@ua.ac.be

10. Prof. Bogdan Bulka, Polish Academy of Sciences, Institute of Molecular Physics, ul. Smoluchowskiego 17, 60-179 Poznan, Poland,
tel: +48 61 8 695 152, fax: +48 61 8 684 524, e-mail: bulka@ifmpan.poznan.pl

11. Prof. Herbert Capellmann, Rheinisch-Westfälische Technische Hochschule, Department of Physics, Sommerfeldstraße, 52074 Aachen, Germany,
tel: +49 241 80 27028, fax: +49 241 80 22188, e-mail: capell@physik.rwth-aachen.de

12. Prof. Jozef Devreese, Department of Physics, Antwerp University, Campus Drie Eiken G.U314, Groenenborgerlaan171, 2610 Antwerpen, Belgium,
e-mail: jozef.devreese@ua.ac.be

13. Prof. Peter Edwards, Department of Chemistry, University of Oxford, South Parks Road, OX1 3QR Oxford, UK,
e-mail: peter.edwards@chem.ox.ac.uk

14. Prof. Konstantin Efetov, Department of Physics, Ruhr-Universität Bochum, Universitätsstraße 150, 44801 Bochum, Germany,
tel: +49 234 32 24844, fax: +49 234 32 14448, e-mail: efetov@tp3.ruhr-uni-bochum.de

15. Prof. Holger Fehske, Ernst-Moritz- Arndt University, Institute for Physics, Am Schießwall 4a, 17487 Greifswald, Germany,
e-mail: fehske@physik.uni-greifswald.de

16. Prof. Yurii A. Firsov, Solid State Physics Division, Ioffe Institute, 26 Polytekhnicheskaya, 194021 St Petersburg, Russia,
e-mail: yuaf@icomefrom.ru

17. Prof. Nicolas Garcia, Consejo Superior de Investigaciones Científicas, Serrano 144, 28006 Madrid, Spain ,
tel : +34 91 563 1774, fax : +34 91 563 1560, e-mail : nicolas.garcia@fsp.csic.es

18. Dr. Martin Hohenadler, Graz University of Technology, Institute for Theoretical and Computational Physics, Petersgasse 16, 8010 Graz, Austria,
tel: +43 316 8738189, fax: +43 316 8738677, e-mail: hohenadler@itp.tu-graz.ac.at

19. Dr. Viktor Kabanov, Jozef Stefan Institute, 1001 Ljubljana, Slovenia,
e-mail: viktor.kabanov@ijs.si

20. Dr. Pavel Kornilovitch, Hewlett-Packard Company, Mail Stop 321A, 1000 NE Circle Blvd., Corvallis, OR 97330, US,
e-mail: pavel.kornilovich@hp.com

21. Prof. Peter Littlewood, Physics Department, University of Cambridge, Madingley Rd., CB3 OHE, Cambridge, UK,
e-mail: pbl21@cam.ac.uk

22. Prof. Ferdinando Mancini, Faculty of Physics, Università degli Studi di Salerno, Via S. Allende, 84081 Baronissi, Italy,
tel: +39 089 965322, fax: +39 089 965275, e-mail: mancini@sa.infn.it

23. Prof. Dragan Mihailovic, Jozef Stefan Institute, 1001 Ljubljana, Slovenia,
e-mail: dragan.mihailovic@ijs.si

24. Prof. Mike Pepper, Physics Department, University of Cambridge, Madingley Rd., CB3 OHE, Cambridge, UK,
e-mail: mp1000@cam.ac.uk

25. Prof. Klaus Ploog, Paul-Drude Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin, Germany,
e-mail: ploog@pdi-berlin.de

26. Prof. Thomas Schimmel, Institut für Angewandte Physik , Universität Karlsruhe, Kaiserstraße 12, 76128 Karlsruhe, Germany,
e-mail : thomas.schimmel@physik.uni-karlsruhe.de

27. Prof. Arndt Simon, Max-Planck Institut für Festkörperforschung, Heisenbergstrasse 1, 70569 Stuttgart, Germany,
e-mail: A.Simon@fkf.mpg.de

28. Prof. Jozef Spalek, Marian Smoluchowski Institute of Physics , Jagiellonian University, Reymonta 4, 30-059 Krakow, Poland,
e-mail: ufspalek@if.uj.edu.pl

29. Prof. Marshall Stoneham, Dept. of Physics and Astronomy , University College London, Gower Street, WC1E 6BT London, UK,
e-mail: a.stoneham@ucl.ac.uk

30. Prof. Carlo Taliani, ISM-CNR, Via P. Gobetti 101, 40129 Bologna, Italy,
e-mail: C.Taliani@ism.bo.cnr.it

31. Prof. Wofgang von der Linden, Graz University of Technology, Institute for Theoretical and Computational Physics, Petersgasse 16, 8010 Graz, Austria,
wvl@itp.tu-graz.ac.at