



Science Meeting – Scientific Report

The scientific report (WORD or PDF file - maximum of seven A4 pages) should be submitted online within two months of the event. It will be published on the ESF website.

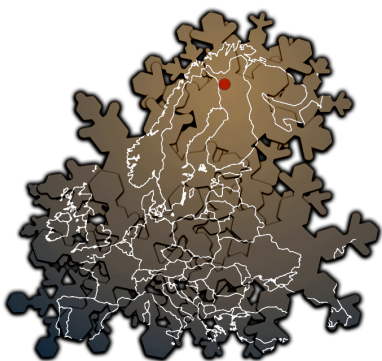
Proposal Title: Towards Reality in Nanoscale Materials VII

Application Reference N°: 5214

- 1) Summary (up to one page)

TRNM VII - Towards reality in nanoscale materials: **Focus on energy materials**

Organizers: Adam S. Foster, Arkady Krashenninikov, Risto Nieminen, Kai Nordlund



The TRNM VII meeting is the seventh in a series of workshops organized in Levi in Finnish Lapland. Although the series maintains a focus on simulations and nanoscale research, each year a new central topic is chosen, and the invited speakers are chosen accordingly. In 2014 the central topic is 'Simulations of Energy Materials', and we had many contributions on this including invited titles such as 'Semiconducting Materials Design by Structural and Chemical Analogy', and 'Engineering thermal and electric transport from first-principles'. Graphene, as expected, was a dominant topic at the meeting in general, but all the studies presented results in keeping with overall theme of *towards reality*.

In total we had over 85 participants at the meeting, continuing the trend of increased numbers every year. The programme was split into 9 invited talks, 24 contributed talks and over 40 posters. In general the meeting was very lively, with good discussion during the presentations, coffee breaks and posters. As always the traditional Lappish dinner makes a good impression and those braving the cold afterwards were rewarded with the Northern lights (we are at 30% observation chance during the history of TRNM). Plans are already being made for TRNM VIII in February 2015.

- 2) Description of the scientific content of and discussions at the event (up to four pages)

The main topics of the workshop were as follows:

- Energy materials – focused on the application of nanoscale investigative techniques, particularly first principles modelling in energy-related research. Including photovoltaics, batteries, [supercapacitors](#), [fuel cells](#), hydrogen technologies, [thermoelectrics](#), [photo- and nanocatalysis](#), solar power technologies, [magnetic refrigeration](#), and [piezoelectric materials](#).
- Graphene and 2D materials – emphasis will be placed on studying the interface of graphene with both adsorbed/deposited nano-objects and underlying substrates.
- Defects - studies of doped and irradiated interfaces and the resultant defect structures. 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 interfaces.
- 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, and the limits of accuracy in electronic structure calculations.
- Multiscale - approaches to link first principles calculations to larger scale methods, such as kinetic Monte Carlo.

The workshop focused on simulations and the majority of the contributions will be from theoretical groups. However, we invited a few experimental experts on selected topics of particular current interest and encouraged abstracts from experimental groups. Further details can be found in the full programme and abstract book attached to this report.

- 3) Assessment of the results and impact of the event on the future directions of the field (up to two pages)

In the 21st century, aggravating energy and environmental problems such as pollution, fossil fuel depletion and global warming are ringing the alarm bell to human society. Therefore, clean and renewable energy materials as well as their devices are urgently demanded, which are the key and foundation to realize the transformation and utilization of new energy. The developments of energy storage and conversion techniques strongly depend on the achievements of material science. Accelerating global energy consumption makes the development of clean and renewable alternative energy sources indispensable. Nanotechnology opens up new frontiers in materials science and engineering to meet this energy challenge by creating new materials, particularly carbon

nanomaterials, for efficient energy conversion and storage. The TRNM workshop covered recent progress in the research and development of materials for advanced energy-conversion devices, including solar and fuel cells, and energy-storage devices, supercapacitors, and lithium-ion batteries, and discusses some challenges in this exciting field.

Computational methods have a long history of applications in the study of materials used in energy technologies and they continue to play a substantial role and one, moreover, which is likely to grow in the future. In particular, modelling of materials at the atomic level is becoming critical - their role is to provide information on the key atomic level structures, processes and parameters that control the behaviour of the material in its applications in either energy generation or storage. Matching with the focus areas of the TRNM workshop, modelling of energy materials makes complete use of the extensive range of techniques available in contemporary condensed matter computational science. Alongside first principles approaches, methods based on interatomic potentials, Monte Carlo and molecular dynamics all have a substantial and continuing role in the field. All will continue to be needed in investigating the complex and varied problems posed by energy materials.

A subset of energy materials, graphene is a two-dimensional (2D) material with a honeycomb-like arrangement of carbon atoms. This is the first truly 2D system with rich physics and chemistry ever manufactured. The isolation and characterization of free-standing graphene sheets had a profound effect on the research of low-dimensional systems, as emphasized by the 2010 Nobel Prize in Physics given to A. Geim and K. Novoselov for its discovery. The peculiar electronic properties and 2D atomic structure make graphene a promising candidate for use in electronics, optoelectronics and photonics. However, the absence of a semiconductor gap in the electronic spectrum (graphene is a semimetal with zero band gap) creates problems for some applications (electronics, light-emitting devices, etc.). This has led to the burgeoning field of 2D materials in general, and this workshop will bring together leading experimental and theoretical efforts. Theoretical data on the dependence of the electronic properties of various mixed and hybrid 2D materials on components composition is largely unknown – particularly with respect to many cutting edge experiments. This knowledge will further be used to assess the possibilities of using mixed 2D materials in various applications. Valuable information on the electronic, and mechanical properties of novel mixed 2D materials will be gained, and this information can be used in designing electronic and optoelectronic devices based on such systems.

Beyond the key thematic areas, TRNM also allowed for methodological presentation and discussion, and at least two sessions devoted to the area – with talks on the latest breakthroughs in first principles simulations and multiscale modelling. At a wider level, the workshop focus areas had impacts on economically and socially important areas such as nanoscience and nanotechnology. In a wider scientific context, TRNM contributed to understanding the fundamental behavior of nanostructured materials and their electronic properties.

4) Annexes 4a) and 4b): Programme of the meeting and full list of speakers and participants

Annex 4a: Programme of the meeting

Annex 4b: Full list of speakers and participants

Programme

	Monday	Tuesday	Wednesday
8:45	<i>Intro</i> <i>chair: Jonsson</i>		<i>chair: Sutter</i>
9:00	Walsh	9:00 Sutter	10:00 Kaiser
9:40	Lasa	9:40 Lehtinen	10:40 Schulz
10:00	Frost	10:00 Herbig	11:00 <i>Coffee</i>
10:20	Pedersen	10:20 Lawlor	<i>chair: Wirtz</i>
10:40	<i>Coffee</i> <i>chair: Csanyi</i>	10:40 <i>Coffee</i> <i>chair: Walsh</i>	11:40 Daraszewicz
11:20	Teobaldi	11:20 Wirtz	12:00 Coutinho
12:00	Gulans	12:00 Hu	12:20 Wallbank
12:20	Musso	12:20 Scardamaglia	12:40 Carva
12:40	El-Sayed	12:40 Carvalho	13:00 <i>Lunch</i> <i>chair: Teobaldi</i>
13:00	<i>Lunch</i> <i>chair: Gulans</i>	13:00 <i>Lunch</i>	16:00 Kiejna
16:00	Csanyi	16:40 <i>Coffee</i> <i>chair: Marzari</i>	16:20 Koskinen
16:40	Heinzel	17:00 Kotakoski	16:40 Jonsson
17:00	Legut	17:40 Seitsonen	17:20 <i>Closing</i>
17:20	<i>Coffee</i> <i>chair: Kiejna</i>	18:00 Abergel	
18:00	Marzari	18:20 <i>Posters</i>	
18:40	Ke	21:00 <i>Dinner</i>	

Contents

Organizers	3
Support	3
Programme	4
Contents	5
Monday	9
Aron Walsh Semiconducting Materials Design by Structural and Chemical Analogy	10
Ane Lasa Multi-scale Modelling of Tungsten Nanosstructure Formation under Helium Irradiation	11
Jarvist Moore Frost Understanding novel thin-film photovoltaic materials . . .	12
Andreas Pedersen Long time scale dynamics of lithium ion cathodes	13
Gilberto Teobaldi Constrained Density Functional Theory in ONETEP: implementation and (innovative?) applications	14
Andris Gulans Pushing the accuracy of electronic-structure calculations to its limits: the exciting code as benchmarking tool	16
Tiziana Musso MoS ₂ /graphene oxide as novel semiconductor/oxide interfaces for electronics	17
Al-Moatasem El-Sayed The nature of intrinsic and extrinsic electron traps in SiO ₂	18
Gabor Csanyi First principles interatomic potentials using machine learning	19
Thomas Heinzl Mechanisms of hydrogen sensing with nanoporous Pt/TiO ₂ diodes	20
Dominik Legut Thermodynamical, optical and mechanical properties of quasi-one-dimensional magnetic phases of KCuF ₃	21
Nicola Marzari Engineering thermal and electric transport from first-principles	22
Xiaoxing Ke Advanced Electron Microscopy on Nanostructures Interface . .	23

Tuesday	25
Peter Sutter Controlled Synthesis of Heterostructures of 2D Materials . . .	26
Ossi Lehtinen Implantation and atomic scale characterization of carbon adatoms in free standing graphene.	27
Charlotte Herbig Ion Irradiation of Metal-Supported Graphene: Exploring the Role of the Substrate	28
James Andrew Lawlor Sublattice asymmetry of substitutionally doped impu- rities in graphene	29
Ludger Wirtz Phonon dispersion and optical properties of layered materials: influence of the environment	30
Ming Hu Abnormal Thermal Transport in Two-dimensional Silicon	31
Mattia Scardamaglia Heavily nitrogen-doped suspended graphene flakes: annealing effects and selectivity of sp^2 nitrogen species	33
Alexandra Carvalho Defect engineering in transition metal dichalcogenide monolayers	34
Jani Kotakoski Atomic structure and electron-beam-driven dynamics of de- fects in graphene	35
Ari Paavo Seitsonen Adsorption of molecules on the h-BN/Rh(111) nanomesh	36
David Stephen Lyne Abergel Excitonic superfluidity in double layer graphene	37
 Wednesday	 39
Ute Kaiser Properties of two-dimensional materials obtained from experi- ments in a low-voltage aberration-corrected TEM	40
Fabian Schulz Modulating the electronic properties of adsorbed molecules by an ultrathin layer of hexagonal boron nitride	41
Szymon Daraszewicz Modelling and probing of non-equilibrium dynamics in irradiated solids	42
José Coutinho Doping and resonant levels from adsorbed molecules to improve the electron mobility of Si-nanocrystal thin films	43
John Wallbank Electronic properties and moiré magnifying effects in graphene on defective hexagonal crystals	44
Karel Carva Magnetic anisotropy energy of thin Fe layers on GaAs surface – the influence of defects	45
Adam Kiejna Fe adsorption on the hematite (0001) and magnetite (111) surface	46
Pekka Koskinen Curvature-controlled valley polarization and band-gap tun- ing in few-layer MoS_2	47
Hannes Jonsson Theoretical studies of the structure and catalytic activity of metallic nanoparticles	48
 Posters	 51
Konstantin Avchaciov Nanoscaled energetic materials with maximum energy density and ductility for self-forming joints in miniaturized systems . .	54

Alexander Bakaev Synergetic Effects of Mn and Si in the Interaction with Point Defects in bcc Fe	55
Vladimir Baturin Structural and electronic properties of small silicon clusters	56
Natalia Berseneva Monolayer boron nitride-graphene heterostructures . . .	57
Carla Bittencourt Nanoscale X-ray Absorption Spectroscopy of isolated BN Nanotubes and ribbons	58
Keith Butler Crystal binding energies of electrons: new strategies for predicting and controlling band energies from first principles	59
Jian-Cheng Chen First principles Kinetic Monte Carlo simulations of the dissolution of NaCl in water	61
Iris Claussen New Milestones in Scanning Probe Microscopy: Graphene on Rh(111) studied by DFT, STM and NC-AFM using KolibriSensor™ and Tyto™	62
Flyura Djurabekova Molecular dynamics simulations of sputtering of a surface under an electric field	63
Robert Drost Revealing Graphene Edge Properties through Interface Engineering	64
Stijn Fias Inducing Aromaticity Patterns and Tuning the Electronic Transport of Graphene Nanoribbons via Edge Design.	65
Jose A. Flores Livas Designing Superhardmagnets From First Principles . .	66
David Gao Multiscale Treatment of Growth and Nucleation of Organic Molecules	67
Fredric Granberg Interaction of dislocations with carbides in BCC Fe	68
Petr Grigorev Benchmarking of interatomic potential for studying of hydrogen – defect interaction in tungsten	69
Soumyajyoti Haldar Designing Fe Nanostructures at Graphene/h-BN Interfaces	70
Ari Harju Anderson localization in disordered graphene: Dimensional crossover and generalized Thouless relation in two dimensions	71
Javad Hashemi Intermediate band photovoltaic cell:	72
Henry Holland-Moritz Enhanced Sputtering effects on ion irradiated Au nanoparticles	73
Sampsa Hämäläinen Where are the atoms? – AFM simulations with a CO terminated tip on corrugated 2D materials	74
Lev Kantorovich On graphene	75
Hannu-Pekka Komsa Electronic structure and optical properties of transition metal dichalcogenide heterostructures	76
Topi Korhonen Quantum and classical elasticity simulations for Graphene spirals	77
Alexander Laikhtman Inorganic Fullerenes And Inorganic Nanotubes Of Tungsten Sulfide For Hydrogen Storage As A Source Of Renewable Energy	78
Aleksi Anssi Leino Mechanism of ion irradiation induced shape transformation of Au nanocrystals	79

Hugo Levard Study of LO-phonon decay in semiconductors for Hot Carrier Solar Cell	80
Claudio Manzato Friction control in nematic system	81
Paulo V C Medeiros The effects of extrinsic and intrinsic perturbations on the electronic structure of graphene: retaining an effective primitive cell band structure by band unfolding	83
Konstantin Mukhin Cryogenic cold neutron moderator for nanostructure research on reactor IBR-2.	84
Tiziana Musso Building realistic models of high-k oxide/semiconductor interfaces	85
Hugo Pinto Adsorption of phosphorus on Pt(111) surface	86
Hugo Pinto The role of surface on the luminescence of the NV centre in diamond	87
Joel Posthuma de Boer A phase field model of irreversible aggregation in submonolayer epitaxial growth	89
Martti Puska Transport studies of metallic carbon nanotube junctions	90
Bernhard Reischl Atomistic simulation of AFM nanoindentation of gold nanoparticles and nanorods	91
Wei Ren MD simulation of DLC-carbon nanotube hybrid materials	92
Ulrike Anne Schröder Etching of Graphene on Ir(111) with Molecular Oxygen	93
Fredrik Silvearv Searching For the Goldilocks Zone In Metal-Carbon Bond Strength for Carbon Nanotube Catalysts	94
Peter Spijker Ionic and organic solid-liquid interfaces as seen by AFM experiments and MD simulations	95
Claudia Struzzi Nitrogen Plasma Functionalization of Vertically Aligned Carbon Nanotubes	97
Dmitry Terentyev Carbon-vacancy complexes controlling radiation damage recovery in Iron	98
Holly Tetlow DFT Calculations of Reactions in Early Stage Graphene Growth	99
John Tracey Modular Python Virtual Atomic Force Microscopy (PyVAFM) . .	100
Ben Xu The first principle study of a new type thermal electric material BiSeCuO	101
Junlei Zhao Molecular Dynamics Simulations of Silver Induced Crystallization in Silicon Nanocluster	102
Sven Öberg Doping and resonant levels from adsorbed molecules to improve the electron mobility of Si-nanocrystal thin films	104

Participants 105

Index 108

Participants

Abergel David Stephen Lyne	Sweden	david.abergel@nordita.org
Avchaciov Konstantin	Finland	konstantin.avchachov@helsinki.fi
Bakaev Alexander	Belgium	abakaev@sckcen.be
Baturin Vladimir	Russia	baturin@lpi.ru
Berseneva Natalia	Finland	natalia.berseneva@aalto.fi
Bittencourt Carla	Belgium	carla.bittencourt@umons.ac.be
Butler Keith	UK	k.t.butler@bath.ac.uk
Carva Karel	Czech Republic	karel.carva@mff.cuni.cz
Carvalho Alexandra	Singapore	physdca@nus.edu.sg
Chen Jian-Cheng	Finland	jian-cheng.chen@aalto.fi
Claussen Iris	Germany	marketing@specs.com
Coutinho José	Portugal	jose.coutinho@ua.pt
Csanyi Gabor	United Kingdom	gc121@cam.ac.uk
Daraszewicz Szymon	UK	szymon.daraszewicz.09@ucl.ac.uk
Djurabekova Flyura	Finland	flyura.djurabekova@helsinki.fi
Drost Robert	Finland	robert.drost@aalto.fi
El-Sayed Al-Moatasem	United Kingdom	ucapabe@live.ucl.ac.uk
Fias Stijn	Belgium	sfias@vub.ac.be
Flores Livas Jose A.	Germany	jaflores@mpi-halle.mpg.de
Frost Jarvist Moore	United Kingdom	j.m.frost@bath.ac.uk
Gao David	UK	david.gao.10@ucl.ac.uk
Granberg Fredric	Finland	fredric.granberg@helsinki.fi
Grigorev Petr	Belgium	pgrigore@sckcen.be
Gulans Andris	Germany	gulans@physik.hu-berlin.de
Haldar Soumyajyoti	Sweden	soumyajyoti.haldar@physics.uu.se
Harju Ari	Finland	ari.harju@aalto.fi
Hashemi Javad	Finland	javad.hashemi@helsinki.fi
Heinzel Thomas	Germany	thomas.heinzel@hhu.de
Herbig Charlotte	Germany	herbig@ph2.uni-koeln.de
Holland-Moritz Henry	Germany	henry.holland-moritz@uni-jena.de
Hu Ming	Germany	hum@ghi.rwth-aachen.de
Hämäläinen Sampsa	Finland	sampsa.hamalainen@aalto.fi
Jonsson Hannes	Iceland	hj@hi.is
Kaiser Ute	Germany	ute.kaiser@uni-ulm.de
Kantorovich Lev	United Kingdom	lev.kantorovitch@kcl.ac.uk

Ke Xiaoxing	Belgium	xiaoxing.ke@untwerpen.be
Kiejna Adam	Poland	kiejna@ifd.uni.wroc.pl
Komsa Hannu-Pekka	Finland	hannu-pekka.komsa@aalto.fi
Korhonen Topi	Finland	topi.korhonen@jyu.fi
Koskinen Pekka	Finland	pekka.koskinen@iki.fi
Kotakoski Jani	Austria	jani.kotakoski@iki.fi
Laikhtman Alexander	Israel	alexl@hit.ac.il
Lasa Ane	Finland	ane.lasa@helsinki.fi
Lawlor James Andrew	Ireland	jalawlor@tcd.ie
Legut Dominik	Czech Republic	dominik.legut@vsb.cz
Lehtinen Ossi	Germany	ossi.lehtinen@uni-ulm.de
Leino Aleksii Anssi	Finland	aleksi.leino@helsinki.fi
Levard Hugo	France	hugolevard@hotmail.fr
Manzato Claudio	Finland	claudio.manzato@aalto.fi
Marzari Nicola	Switzerland	nicola.marzari@epfl.ch
Medeiros Paulo V C	Sweden	paume@ifm.liu.se
Mukhin Konstantin	Russia	kostik001@mail.ru
Musso Tiziana	Finland	tiziana.musso@aalto.fi
Pedersen Andreas	Switzerland	andreas@hi.is
Pinto Hugo	Finland	hugo.pinto@aalto.fi
Posthuma de Boer Joel	England	jp611@ic.ac.uk
Puska Martti	Finland	martti.puska@aalto.fi
Reischl Bernhard	Finland	bernhard.reischl@helsinki.fi
Ren Wei	Finland	wei.ren@helsinki.fi
Scardamaglia Mattia	Belgium	mattia.scardamaglia@umons.ac.be
Schröder Ulrike Anne	Germany	schroeder@ph2.uni-koeln.de
Schulz Fabian	Finland	fabian.schulz@aalto.fi
Seitsonen Ari Paavo	Switzerland	ari.p.seitsonen@iki.fi
Silvearv Fredrik	Sweden	fredrik.silvearv@ltu.se
Spijker Peter	Finland	peter.spijker@aalto.fi
Struzzi Claudia	Belgium	claudia.struzzi@gmail.com
Sutter Peter	USA	psutter@bnl.gov
Teobaldi Gilberto	UK	g.teobaldi@liv.ac.uk

Terentyev Dmitry	Belgium	dterenty@sckcen.be
Tetlow Holly	UK	holly.tetlow@kcl.ac.uk
Tracey John	Finland	john.tracey@aalto.fi
Wallbank John	United Kingdom	j.wallbank@lancaster.ac.uk
Walsh Aron	UK	a.walsh@bath.ac.uk
Wirtz Ludger	Luxembourg	ludger.wirtz@uni.lu
Xu Ben	China	xuben@mail.tsinghua.edu.cn
Zhao Junlei	Finland	junlei.zhao@helsinki.fi
Öberg Sven	Sweden	sven.oberg@ltu.se