Research Networking Programmes

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.

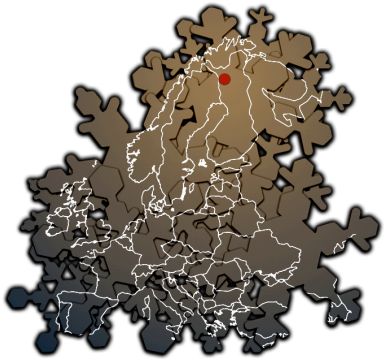
***Proposal Title*: Towards Reality in Nanoscale Materials VII**

***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 TRMN 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	
8:45	*Intro*
	chair: Jonsson
9:00	**Walsh**
9:40	Lasa
10:00	Frost
10:20	Pedersen
10:40	*Coffee*
	chair: Csanyi
11:20	**Teobaldi**
12:00	Gulans
12:20	Musso
12:40	El-Sayed
13:00	*Lunch*
	chair: Gulans
16:00	**Csanyi**
16:40	Heinzel
17:00	Legut
17:20	*Coffee*
	chair: Kiejna
18:00	**Marzari**
18:40	Ke

Tuesday	
	chair: Kaiser
9:00	**Sutter**
9:40	Lehtinen
10:00	Herbig
10:20	Lawlor
10:40	*Coffee*
	chair: Walsh
11:20	**Wirtz**
12:00	Hu
12:20	Scardamaglia
12:40	Carvalho
13:00	*Lunch*
16:40	*Coffee*
	chair: Marzari
17:00	**Kotakoski**
17:40	Seitsonen
18:00	Abergel
18:20	*Posters*
21:00	*Dinner*

Wednesday	
	chair: Sutter
10:00	**Kaiser**
10:40	Schulz
11:00	*Coffee*
	chair: Wirtz
11:40	Daraszewicz
12:00	Coutinho
12:20	Wallbank
12:40	Carva
13:00	*Lunch*
	chair: Teobaldi
16:00	Kiejna
16:20	Koskinen
16:40	**Jonsson**
17:20	*Closing*

Contents

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 Aleksi 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