

Towards Reality in Nanoscale Materials V

20th — 22nd February 2012
Levi, Lapland, Finland

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Organizers

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Acknowledgement for financial support

European Science Foundation

Psi-k Network

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Report

The Towards Reality in Nanoscale Materials V workshop was the fifth in this annual series, although its origins can be traced to a meeting on wet chemical etching in Levi in 2006. Each year the focus changes, with one key topic supported by the regular themes of defects and multiscale modelling, all under the umbrella of nanoscale materials. This year's key topic was graphene interfaces, and we had many contributions on this including invited titles such as 'Graphene on metal surfaces', and 'Quantum confined electronic states in atomically well-defined graphene nanostructures'. 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 80 participants at the meeting, continuing the trend of increased numbers every year. The programme was split into 9 invited talks, 25 contributed talks and 48 posters. Unlike the chaos caused last year by a Finnair strike, we lost only four participants at the last minute - two to the snow in Sweden, one to thieves in Italy and one mysteriously in Turkey. In general the meeting was very lively, with good discussion during the presentations, coffee breaks and posters. The switch of the meeting from the dark of December to February was a major bonus, as we actually had daytime rather than just twilight/night this year. 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 50% observation chance during the history of TRNM). Plans are already being made for TRNM VI in February 2013.

Programme

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|--------------|-------------------|----------------|----------------|
| 8:45 | intro | | |
| <i>chair</i> | <i>Rinke</i> | <i>Roche</i> | <i>Busse</i> |
| 9:00 | Artacho | Busse | Roche |
| 9:40 | Bøggild | Lehtinen | Ahlskog |
| 10:00 | Sob | Pietrucci | Makarova |
| 10:20 | Borlenghi | Booth | Carva |
| 10:40 | <i>coffee</i> | <i>coffee</i> | <i>coffee</i> |
| <i>chair</i> | <i>Pantelides</i> | <i>Perez</i> | <i>Artacho</i> |
| 11:20 | Watkins | Liljeroth | Pantelides |
| 12:00 | Barth | Ewels | Minato |
| 12:20 | Laasonen | Amara | Girard |
| 12:40 | Rayson | Kurasch | Uppstu |
| 13:00 | <i>lunch</i> | <i>lunch</i> | <i>lunch</i> |
| <i>chair</i> | <i>Liljeroth</i> | | <i>Bøggild</i> |
| 16:00 | Rinke | <i>posters</i> | Sinnott |
| 16:40 | Susi | 16:00 – 18:00 | Mittendorfer |
| 17:00 | Standop | | Perez |
| 17:20 | <i>coffee</i> | | |
| <i>chair</i> | <i>Sinnott</i> | | closing |
| 18:00 | Chamberlain | <i>dinner</i> | |
| 18:20 | Björk | 18:00 – 21:00 | |
| 18:40 | Philipp | | |

- Monday
 - Emilio Artacho: Origin of the 2DEG at oxide interfaces, relation with topology and with redox defects, and possible 1DEG
 - Peter Boggild: On chip synthesis and characterisation of nanostructures in-and outside TEM
 - Mojmir Sób: Ab initio study of mechanical and magnetic properties of Mn Pt compounds and nanocomposites
 - Simone Borlenghi: Electronic transport and magnetization dynamics in realistic devices:a multiscale approach
 - Matthew Watkins: Developing realistic models of interfaces from simulation
 - Clemens Barth: Two-dimensional growth of nanoclusters and molecules on Suzuki surfaces
 - Kari Laasonen: Reaction studies of Al-O clusters in water
 - Mark Rayson: Towards large-scale accurate Kohn-Sham DFT for the cost of tight-binding
 - Patrick Rinke: Towards a unified description of ground and excited state properties:RPA vs GW
 - Toma Susi: Core level binding energies of defected and functionalized graphene
 - Sebastian Standop: Spatial Analysis of Ion Beam induced Defects in Graphene
 - Thomas Chamberlain: Utilizing carbon nanotubes as nanoreactors
 - Jonas Björk: Molecular self-assembly of covalent nanostructures: Unraveling their formation mechanisms
 - Patrick Philipp: Simulation of defect formation and sputtering of Si(100) surface under low-energy oxygen bombardment using a reactive force-field

- Tuesday
 - Carsten Busse:Graphene on metal surfaces
 - Ossi Lehtinen: Detailed structure and transformations of grain boundaries in graphene
 - Fabio Pietrucci: Graph theory meets ab-initio molecular dynamics: atomic structures and transformations at the nanoscale
 - Tim Booth: Discrete removal of carbon atoms by silver nanoparticles in suspended graphene

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- Peter Liljeroth: Quantum confined electronic states in atomically well-defined graphene nanostructures
 - Chris Ewels: Distorting graphene through mechanics and edge chemistry
 - Hakim Amara: Healing Mechanisms During The Growth of Carbon Nanotubes
 - Simon Kurasch: Graphene: An ideal substrate for TEM imaging and spectroscopy
 - Wednesday
 - Stephan Roche: Transport Properties in Disordered Graphene: Effects of Atomic Hydrogen and Structural Defects
 - Markus Ahlskog: Size dependence of electronic transport in multi-walled carbonnanotubes
 - Tatiana Makarova: Edge states versus in-plane defects in graphite magnetism
 - Karel Carva: Defect controlled conductivity of graphene with vacancies and N impurities
 - Sokrates Pantelides: Topics in graphene
 - Taketoshi Minato: Mechanism of organic chemical reactions on nanoporous gold
 - Sylvain Girard: Coupling experiments and simulations for the radiation hardening of fiber optics: (I) Experimental results on canonical samples of pure and doped silica
 - Andreas Uppstu: Electronic transport in graphene-based structures: An effective cross section approach
 - Susan Sinnott: Charge Optimized Many-Body (COMB) Potentials for Interfacial Studies
 - Florian Mittendorfer: Graphene on Ni(111): Strong Interaction and Weak Adsorption
 - Ruben Perez: Probing nanostructures with forces and currents: From atomic-scale contrast on graphene and carbon nanotubes to hetero-fullerene synthesis with planar aromatic precursors
 - Posters
 - Harriet Ahlgren: Ion irradiation induced defects in freestanding graphene: an atomistic simulation study
 - Hadi Arefi: A density functional theory study of functionalised silicon surfaces

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- Joseph Bamidele: The role of dispersion forces in the surface stability of oxidised Cu(110)
 - Vladimir Baturin: On heat capacity of superconducting nanoclusters
 - Carla Bittencourt: Imaging the carbon K near-edge polarization dependence of a few layer graphene by NEXAFS-TXM
 - Alexandra Carvalho: Alternative methods for doping nanocrystals and designing junction offsets
 - Vladimir Chashchikhin: DFT modeling of the interaction of small analyte molecules with a dye/silica receptor center
 - Filippo Federici: NC-AFM energy dissipation mechanisms
 - Filippo Federici: Atomic scale dynamics of frictional processes
 - Filippo Federici: Extreme sensitivity in potential characterization of an insulating step edge
 - Yulia Filicheva: Theoretical investigation of the diamond films with implanted oxygen atoms
 - Andris Gulans: From short- to long-range correlations in layered materials
 - Eero Holmström: Atomic-scale processes set the critical limit for conventional ion beam thinning of Silamellae
 - Semran Ipek: Structural and electronic properties of GaAs nanotubes
 - Elisa Jimenez: Porous Solids Based on Endohedrally Doped CdS Nanoclusters
 - Wonjae Kim: Nonlinear behavior of three terminal graphene junctions at room temperature
 - Manana Koberidze: Molecular Dynamics Simulation of Aluminum Oxidation via Reactive Force Field
 - Hannu-Pekka Komsa: Defects in electron irradiated transition metal dichalcogenides
 - Jaap Kroes: Atomic oxygen chemisorption on a zig-zag carbon nanotube
 - Sampo Kulju: Atomic scale characterization of alumina films grown on the MgAl₂O₄(100) surface
 - Alexander Kvashnin: Ultrathin diamond nanofilms as possible two-dimensional insulator: electronic and elastic properties
 - Dmitry Kvashnin: Transport properties of graphene-based branched nanoribbons. Theoretical study
 - Katri Laaksonen: Optical properties of thermochromic VO₂ nanoparticles

- Markus Langer: Imaging and energy dissipation mechanisms on metallic and insulating surfaces studied with AFM in pendulum geometry
- Nikita Marchenkov: Lattice parameter local determination for trigonal crystal systems using several coplanar X-ray reflections
- Taketoshi Minato: Atomic defects on titanium dioxide surface -Electronic structure and manipulation
- Riku Oja: d0 ferromagnetic interface between non-magnetic perovskites
- Ari Ojanpera: Ehrenfest molecular dynamics within the projector augmented-wave method: an ab initio insight on electronic stopping in nanostructures
- Alexander Pyymaki Perros: Interfacial characteristics of in situ CVD-seeded ALD oxide layers on graphene
- Filippo Pizzocchero: Direct density functional theory simulation of single sequential transmission electron microscope images
- Nicolas Richard: Coupling experiments and simulations for the radiation hardening of fiber optics: (II) Ab initio characterization of electronic and optical properties of defects in amorphous silica
- Juho Roukala: Magnetic resonance properties of Sc₃C₂@C₈₀ in finite temperatures
- Arto Sakko: Time-dependent DFT approach for the dielectric response of nanoscale systems
- Karri Saloriotta: Resonant scattering in graphene: adsorbate fingerprints from ab initio calculations
- Nino Samadashvili: Nanoscale friction of ice
- Dmitri Schebarchov: Interplay of geometric and electronic structure in metalloid gallium clusters
- Martha Scheffler: Local tunneling spectroscopy of the Hydrogen-induced impurity state in quasi-freestanding graphene
- Gabriele Sclauzero: Corrugation-enhanced graphene reactivity boosting the graphene/SiC(0001) interface stability
- Anton Targonsky: New Method for Measuring Rocking Curves in X-Ray Diffractometry for time resolving observation of the crystal defects by Ultrasonic Modulation of the Lattice Parameter
- Stefan Taubert: Molecular dynamics simulations of initial stages of growth of nitrogen-doped carbon nanotubes
- Dmitry Terentyev: Modelling of radiation damage recovery in concentrated Fe-Cr alloys: a multi-scale modelling approach
- Lisa Katharina Tschammer: Nanomanipulation of Graphene using E-beam and Block Copolymers

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- Jarkko Vahakangas: NMR parameter of chemically modified graphanes
 - Ville Virkkala: Hybrid-Functional Study of Band-Structures of GaAs_xN_x and GaSb_xN_x Alloys
 - Monika Vsianska: The effect of non-magnetic impurities on magnetic and cohesive properties of grain boundaries in nickel
 - Valeria Zagaynova: Influence of boron doping on the defect-induced magnetism of oxygen-eroded graphite
 - Martin Zeleny: First-principles investigation of the martensitic transformation in Co-doped Ni₂MnGa shape memory alloys

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