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REPORT
for the 88th IUVSTA Workshop "Towards Reality in Nanoscale Materials"

Background and outcome

The 88th workshop was organized under the sponsorships of Aalto University, TSV Federation and the IUVSTA Nanometer Structures Division with the support of the Electronic Materials and Process Division and Surface Engineering Division on 12-14 February 2019 in Levi, Finland. The workshop was jointly organized by Prof. Adam Foster, Aalto University, Dr. Carla Bittencourt, University of Mons, Belgium, Dr. Arkady Krasheninnikov, Helmholtz-Zentrum Dresden-Rossendorf, Germany and Aalto University, Finland and Dr. Teemu Hynninen, University of Turku, Finland. Prof Foster and Dr. Hynninen acted as local organizers.

The main idea behind this workshop was 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 defects and irradiation effects in various nanoscale materials, including carbon nanomaterials, such as graphene. Considerable attention has also been given to surface probe methods. The lectures given by the experts in simulations of irradiation effects in nanomaterials such as carbon and boron-nitride nanotubes, graphene, small metal clusters etc., were combined with those presented by the developers of the relevant simulation methods (e.g., time-dependent density-functional theory, molecular dynamics algorithms). In addition to the theoretical advances, recent progress in experiments were covered by several speakers. The latest and most important results in the field were presented by the speakers and during the poster session. In addition to recently published results, a considerable amount of new unpublished data was presented. The central point was the role of defects in the behavior of nanosystems and related issues such as the production of defects under electron and ion irradiation, the characterization of defects by various techniques, and finally the beneficial aspects of defects in engineering the properties of nanosystems and in nano-scale catalysis. Such a combination of complementary topics (theory/experiment, theoretical method development/applications etc.) resulted in interesting and productive scientific discussion which should have a strong impact on the development of the field and could eventually give rise to new scientific collaborations. Due to a considerable number of students and

young postdocs from EU countries who participated in the workshop (about 50% of the attendees), the event was also important in the context of training of young researchers. Overall, based on the response we received from the participants, the workshop was a success opening avenues for a series of workshops in scientific complementary fields.

The workshop website will be maintained so detailed information will be accessible via: http://trnm.aalto.fi/

Workshop participants

The workshop was attended by 58 participants (including the organizers). This number was given by limitation of the venue, the number of people who expressed interest was close to 80. The participants were from all over the World (10European countries + USA, China, Russia). The interaction among all participants was very dynamic making possible the establishment of new scientific collaborations.

Workshop scheme

The 4 days long workshop started at Monday evening with a welcome reception and closed Thursday afternoon. The workshop was divided in 7 topical sections:

- Tools - focused on recently developed methods for nanoscale characterization and integration with bulk materials.
- Applications - nanoelectronics sensors, catalysis for decontamination of water, land and objects.
- 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.
- 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.
- Transport - studies of the migration of defects, impurities and electrons across interfaces.

The workshop consisted of invited and contributed talks as well as posters. Invited and contributed speakers covered the recent progress in simulations and the relevant experimental areas. Altogether, there have been 32 talks and 20 posters. The regular contributed talks were 20 min long while the invited were 40 minutes long. Additionally, at the end of each day, there was a ´Summary of the day´ session which was aimed to

discuss recent progress on characterization of defects on nanostructures (both theoretical and experimental) in order to share the state-of-the-art in the field, identify accomplishments and discuss challenges and opportunities.

The venue was a scenic spot in Lapland during the winter which provided all the comfort and quietness needed for an intense workshop. We were rewarded with a strong Aurora borealis display.

Financial

The workshop fee included hotel accommodation (4 nights + 4 breakfasts + 3 lunches + 1 banquet + many coffees), the workshop dinner was in the restaurant Saamen Kammi. Fees depended on the type of the chosen accommodation: shared room in a skiing house (chalet): 340 €, own room in a skiing house (chalet): 500 €, own hotel room: 130 €/night + 70 € for banquet.

The Beilstein Institute provided conference bags. The incoming amount of money was 43306 EURO, including the IUVSTA contribution of 6000 EURO, 9000 by TSV Federation (Finland) and 2000 by Aalto University; the workshop fee of invited scientists was waived.

The 88th IUVSTA Workshop "Towards Reality in Nanoscale Materials" organizers

Carla Bittencourt

Adam Foster

Teemu Hynninen

Arkady Krasheninnikov

Budget for the Workshop (2016.10.24-28)

TITLE: IUVSTA Workshop on Towards Reality in Nanoscale Materials
VENUE: Levi, Finland
DATE: 12 – 14 February 2019

Income	Unit cost (EUR)	Quantity	Sub-Total (EUR)	Remarks
Registration Fee	24.780	1	24.780	
Extra expenses of accompanying person	1.526	1	1.526	
TSV Federation (Finland)	9.000	1	9.000	
AAlto funding	2.000	1	2.000	
IUVSTA funding	6.000	1	6.000	
Total (EUR)			43.306	

Expenditures	cost (EUR)	Quantity	Sub-Total (EUR)	Remarks
Hotel	38.896	1	38.896	Rent of chalets to accomodate the participants, Conference Facilities (lecture hall and poster session), Lunches and Coffee breaks
Banquet	940	1	940	
Abstract book	500	1	500	
Travel (inv. Speakers)	2.970	1	2.970	
Total (EUR)			43.306	