Conference on Physics of Defects in Solids: Quantum Mechanics Meets Topology

9 - 13 July 2018
Trieste, Italy

Electronic Abstract Book

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ICTP - The Abdus Salam International Centre for Theoretical Physics

Kastler Lecture Hall (AGH)
Via Grignano, 9 I - 34151 Trieste (Italy)

https://defectsinsolids.wordpress.com/

http://indico.ictp.it/event/8321/

Welcome

Defects in crystalline solids are ubiquitous. It is the second law of thermodynamics that gives rise to the appearance of a certain amount of disorder in crystalline materials at finite temperatures. Moreover, defects can be present in synthetic materials well above the equilibrium concentration due to the imperfections of material production processes or due to the exposure of the system to irradiation with energetic particles. Such lattice imperfections have a strong influence on the electronic, optical, thermal, and mechanical properties of the solids, normally deteriorating their characteristics.

However, defects not always have detrimental effects on material properties, with the most prominent example being the doping of semiconductors by controllable introduction of impurities using ion implantation. In general, treatments of solids with beams of energetic ions and electrons have been shown to be a very powerful tool for the post-synthesis tailoring of material characteristics.

The goal of the conference is to bring together active researchers in the field, as well as several experts in the related areas, to discuss "state of the art" in theory and experiment dealing with the physics of defects in solids. The effects of impurities and point/line defects on various properties of solids will be addressed, and the attendees will be able to learn not only the experimental facts, but also understand how the defects are treated within the framework of computational and analytical methods in theoretical physics. Particular attention is going to be paid to defects in nanomaterials, as the reduced dimensionality strongly affects their behavior.

We are particularly grateful to the ICTP for hosting this meeting, and its help both financially and with the conference organization. We would also like to thank our co-sponsors, Aalto Univesrity, the FNRS, the Helmholtz Zentrum Dresden Rossendorf (HZDR), Scientaomicron, and Zurich Instrucments. Without their support this conference could not have happened.

We hope you enjoy your week with us, and have an interesting and scientifically stimulating meeting.

The Conference Organisers.

Practical Information
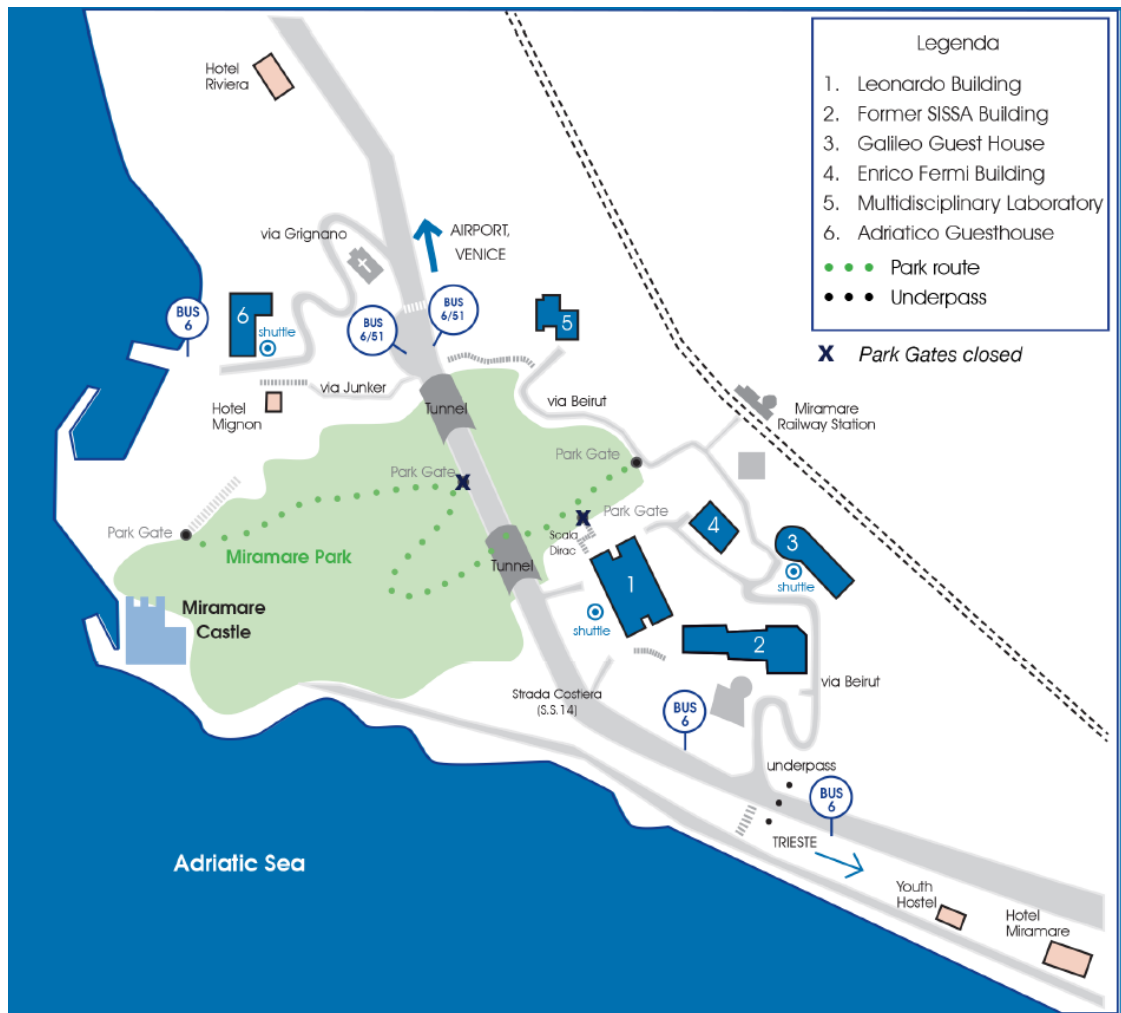
Many participants are staying at the [Adriatico Guesthouse](#), on the ICTP campus, in Miramare. The conference takes place at the [Kastler Lecture Hall](#), in the Lower Level 1 inside the Adriatico Guesthouse. In addition to the lecture halls and rooms, the guest house has a reception office, the cafeteria, a reading room, a TV lounge, vending machines and a laundry room.

All financially supported participants lodging at ICTP Guesthouses should visit the Operations and Travel Unit at the Enrico Fermi Building in order to fulfill all financial procedures. Please bring your passport and travel receipts. Registration is at the Adriatico Guesthouse Lower Level, this is only for participants lodging outside ICTP premises and faculty.

A branch office of Unicredit Banca is located at the Enrico Fermi Building, next to the entrance hall, on the ground floor.   This has an ATM (cash machine).   The best way to get to central Trieste is by bus. Right in front of the guest house is the last stop of bus #36. You must purchase your ticket before you get on. These can be purchased at the reception desk inside the Adriatico Guesthouse (cash only).

More practical details are available [here](#) and [here](#).

Programme

Please note that the [full programme is available online](#) including links to slides where available.

Internet Access

In order to connect your laptop to the ICTP from a **guest room** of the AGH or GGH, you need a **network cable of your own**. In or near most computer labs there are desk spaces dedicated to laptop users. There you will find network cables ready to use, permanently attached to the network outlets.

Firewall restrictions: For security reasons there are many network restrictions. One of them is relevant for people using a VPN (Virtual Private Network) to connect to their home institutions. All such connections must be initiated from within the ICTP. We cannot allow connections to be initiated from outside.

You cannot directly connect to external computers using the standard HTTP port 80. Our **proxy server** must be used for this purpose. Either use automatic proxy detection, or set the automatic configuration script to http://wpad.ictp.it/wpad.dat, or manually configure to proxy.ictp.it, port 3128.

Wireless network

Eduroam is available from the ICTP.

There is also two specific wireless networks at the ICTP. They use WPA and require that the software driver for your wifi card is fairly recent, so you might need to update it from the manufacturer's web site. You need to have your ICTP account information ready. You will get it from the secretary of your workshop or hosting scientific group during the registration process. To connect to **ictp-secure**, you may need to enter: Security-Type: WPA2-Enterprise, Encryption-Type: AES, EAP-Type: Protected EAP (PEAP), Phase-2-authentication/authentication-method: MSCHAPv2, anonymous-identity: leave blank, server-certificate: none (disable verification).

Use **ictp-open** only if you cannot connect to the other two. No setup is needed but everytime you reconnect you will have to enter the credentials through a web page before you get access to the Internet.

Organizers

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Sponsors

We are grateful to our sponsors for their support of this event:

Programme

Monday
9 July

08:30   Registration, Administrative and Financial formalities

All financially supported participants lodging at ICTP Guesthouses should visit the Operations and Travel Unit at the Enrico Fermi Building in order to fulfill all financial procedures. Please bring your passport and travel receipts. **Registration at Adriatico Guesthouse Lower Level:** *only for participants lodging outside ICTP premises and faculty.*

09:00 Tutorial   A. Krasheninnikov (Helmholtz-Zentrum Dresden-Rossendorf, Germany
                        and Aalto University, Finland)
                   Defects in bulk and low-dimensional materials

09:30 Tutorial   T. Michely (University of Köln, Germany)
                   Identification of surface defects using STM

10:00 Tutorial   T. Susi (University of Vienna, Austria)
                   Identifying defects using transmission electron microscopy and spectroscopy

10:30 Tutorial   H.-P. Komsa (Aalto University, Finland)
                   Atomistic modeling of point defects

11:00 Coffee break

11:30 Tutorial   M. Nastasi (University of Nebraska at Lincoln, USA)
                   Ion-Solid Interactions and Defect Formation

12:00 Tutorial   A. Vantomme (KU Leuven, Belgium)
                   Assessing defects in solids with ion channeling

12:30 Tutorial   M. Scardamaglia (University of Mons, Belgium)
                   Recent developments in x-ray photoelectron spectroscopy

13:00 Lunch break

15:00 - 17:00 Session 1   Chair: A. Krasheninnikov

15:00   T. Michely (University of Köln, Germany)
                   Luttinger liquid in a box: electrons confined within MoS_2 mirror twin boundaries

15:40   J. Neugebauer (Max-Planck-Institut für Eisenforschung, Germany)
                   First-principles approaches for charged defects in low dimensional systems

16:20 Coffee break

17:00 - 18:20 Session 2   Chair: D. Efremov

17:00   L. Pizzagalli (CNRS, France)
                   Dislocations in covalent materials: the puzzling complexity of cores

17:40   G. Astakhov (Helmholtz-Zentrum Dresden-Rossendorf, Germany)
                   Engineering of spin defects in silicon carbide for quantum applications

18:20   D. Kvashnin (National University of Science and Technology MISiS, Russian Federation)
                   High Oxygen Doping of h-BN for Electronic and Magnetic Properties Engineering

19:30 - 21:30 Welcome Reception

All participants of the Conference are cordially invited to the Welcome Reception.
Location: Adriatico Guesthouse – Terrace

Defects in Bulk and Low-Dimensional Materials

Arkady V. Krasheninnikov [1,2,3,4]

[1]Helmholtz Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Germany
[2]Department of Applied Physics, Aalto University School of Science, Finland
[3]DTU Nanotech, Technical University of Denmark, Lyngby, Denmark
[4]National University of Science and Technology MISiS, 119049 Moscow, Russia.

Defects in crystalline solids are ubiquitous. It is the second law of thermodynamics that gives rise to the appearance of a certain amount of disorder in crystalline materials at finite temperatures. Moreover, defects can be present in synthetic materials well above the equilibrium concentration due to the imperfections of material production processes or due to the exposure of the system to irradiation with energetic particles. Such lattice imperfections have a strong influence on the electronic, optical, thermal, and mechanical properties of the solids, normally deteriorating their characteristics.

However, defects not always have detrimental effects on material properties, with the most prominent example being the doping of semiconductors by controllable introduction of impurities using ion implantation. In general, treatments of solids with beams of energetic ions and electrons have been shown to be a very powerful tool for the post-synthesis tailoring of material characteristics.

In my talk, I will present the "state of the art" in theory and experiment dealing with the physics of defects in solids. The effects of impurities and point/line defects on various properties of solids will be addressed, and not only the experimental facts will be presented, but also the computational and analytical methods used in theoretical physics to get insights into defect behavior. Particular attention is going to be paid to defects in nanomaterials, as the reduced dimensionality strongly affects their behavior. Specifically, I will present the results [1] of our first-principles theoretical studies of defects (native and irradiation-induced) in inorganic 2D systems obtained in close collaboration with several experimental TEM groups. I will further discuss defect- and impurity-mediated engineering of the electronic structure of inorganic 2D materials. I will also present the results of our theoretical studies of electron-beam induced phase transformations in 2D TMDs when electric charge, mechanical strain and vacancies are present. Based on the results of our calculations, we propose an explanation for this phenomenon which is likely promoted by charge redistribution in the monolayer combined with vacancy formation due to electron beam and associated mechanical strain in the sample.

[1] http://users.aalto.fi/~ark/publist.html .

Identification of surface defects using STM

Thomas Michely

II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany

After considering the basic modes of operation of scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS), a number of examples for defect identification will be discussed. These range from identification of defect structure and their function in surface reactions over ion induced defects to the identification of changes in the electronic structure induced by defects.

One surprising consequence of the presence of point defects at a surface is that point defects may serve to determine the electronic structure of the undisturbed material.

Identifying defects using transmission electron microscopy and spectroscopy

T. Susi

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In this tutorial, I will introduce (scanning) transmission electron microscopy and show how it can identify the atomic structure of defects [1]. In combination with electron energy loss spectroscopy [2], the chemical identity and even bonding of impurities such as heteroatom substitutions in graphene can be unambiguously determined [3,4]. Since the energetic imaging electrons carry significant momentum, damage by the electron beam must also be considered [5], and in some cases, purposefully used for single-atom manipulation [6,7].

[1] O.L. Krivanek *et al.*, Nature 464 (2010) 571.
[2] R.F. Egerton, Reports on Progress in Physics 72 (2009) 016502.
[3] Q.M. Ramasse *et al.,* Nano Lett. 13 (2013) 4989.
[4] T. Susi *et al.*, 2D Materials 4 (2017) 021013.
[5] R.F. Egerton *et al.*, Ultramicroscopy 110 (2010) 991.
[6] T. Susi *et al.,* Ultramicroscopy 180 (2017) 163.
[7] T. Susi *et al.*, arXiv:1803.05338 (2018).

Atomistic modeling of point defects

H.-P. Komsa[1]

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In this tutorial, a brief introduction to first-principles calculations within density functional theory is given, followed by its application to point defect calculations. The focus is on the calculation of formation energies, charged defects, and defect levels, while paying attention to the limitations of the underlying computational framework.

Ion-Solid Interactions and Defect Formation

Michael Nastasi

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mnastasi2@unl.edu

This tutorial will focus on ion irradiation and defect formation in solids. Sources of ion irradiation will be discussed. Ion implantation will be used as a model system for ion-solid interaction. We will explore the concept of ion stopping in materials and how energy deposition into the nuclear system of the solid result in the production of atomic displacements and defect formation.

Assessing defects in solids with ion channeling

A. Vantomme

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From the energy loss during scattering of high-energy, light ions from a solid, the compositional depth profile of the near-surface region can be easily deduced. Indeed, conservation of energy and linear momentum during the scattering event, along with the scattering cross section as derived by Ernst Rutherford more than a century ago, allow determining the mass of the atomic species in the sample (hence identifying them), their concentration as well as their depth. These physics principles constitute the basics of *Rutherford backscattering spectrometry*, a technique which is routinely used in materials science and solid-state physics.

When dealing with single crystalline samples, the alignment of the impinging ion beam with a high-symmetry direction of the crystal (i.e., an axis or a plane) can result in a drastic reduction of the backscattering yield, while leaving the mass and depth dependence unaffected – a phenomenon referred to as *ion channeling* [1, 2]. From this yield reduction and its angular dependence, valuable information can be obtained on the crystal structure and any deviation from its ideal crystallinity. In other words, ion channeling allows investigating a wide variety of defects in single crystals.

In this tutorial, an overview will be given of the basics of RBS and channeling, and how these techniques can be used to assess defects, mainly focusing on lattice disorder (point defects and alike) and the lattice site of impurities in a crystal.

[1] L.C. Feldman, J.W. Mayer and S.T. Picraux, Materials Analysis by Ion Channeling (Academic Press, NY), 1982.
[2] A. Vantomme, Nucl. Instr. Meth. B 371 (2016) 12.

Recent developments in x-ray photoelectron spectroscopy

M. Scardamaglia

University of Mons - Belgium

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In this tutorial, an overview of x-ray photoelectron spectroscopy (XPS) will be given. Through examples focused on the analysis of defects in graphene, we will explain how useful is the XPS for the determination of the chemical environment on a specimen.
We will review standard lab- and synchrotron-based techniques and show recent developments to achieve spatial resolution and ambient pressure experiments.

Luttinger liquid in a box: electrons confined within MoS$_2$ mirror twin boundaries

Thomas Michely

II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany

While in two or three dimensional metals low-energy excitations and properties are usually well described by weakly interacting fermionic quasiparticles, in one dimension this concept breaks down due to strong Coulomb interactions. In one dimensional (1D) metals, the low-energy excitations are expected to be independent spin- and charge density waves, as described by the Tomonaga-Luttinger liquid theory. Experimental research on the physics of 1D metals is still hampered by their difficult preparation, by competing or covering effects like Peierls type charge density waves or disorder induced zero bias anomalies, and by limitations in our experimental tools. Here we construct a rather perfect 1D metal of finite length using a specific defect in a transition metal dichalcogenide monolayer, namely a mirror twin boundary in layer of MoS$_2$. The layer itself is well decoupled from the environment and rests on graphene on Ir(111). We use scanning tunneling microscopy and spectroscopy to obtain unique fngerprints of spin-charge separation in real space by measuring the probability distribution and energy of quantum mechanical states in a 1D box. The interpretation of our data is based on the fact that for a Tomonaga-Luttinger liquid in a box the local distribution of the single-particle spectral weight - determining the probability to inject or extract an electron in a tunneling experiment – visualizes its fundamental properties. We critically discuss our results in the light of previous related research.

First-principles approaches for charged defects in low dimensional systems

Christoph Freysoldt[1], Michael Ashton, <u>Jörg Neugebauer[1]</u>

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Charged defects at surfaces, interfaces, or 2D materials strongly affect the behavior of bulk or nanostructured semiconductor materials. Being able to tune this behavior is central to various technological applications: in electronic and optoelectronic devices, in chemical sensors, or in electrochemistry and corrosion. To achieve this level of control it is necessary to determine the defects' thermodynamic and electronic properties. Significant progress has been made in recent years in calculating formation energies of point defects within bulk materials from first-principles electronic-structure calculations. However, charged defects in and at low dimensional structures pose severe challenges to theoretical modelling.

We have therefore developed two methodologies that allow to use standard DFT codes to efficiently compute electronic, structural, and energetic properties of charged defects in low dimensional systems. One approach allows to include macroscopic internal electric fields as present in electronic devices due to applied biases or depletion zones. The other allows to study the formation and the properties of defects created under the influence of extreme electric fields as e.g. present in modern experimental techniques with atomic resolution (field ion microscopy, atom probe tomography). Both methods converge rapidly with supercell size and allow to get converged formation energies in the isolated defect limit independent of vacuum thickness, slab thickness, or lateral supercell size. The performance of these approaches is demonstrated for defects on various semiconductor surfaces and for describing defect creation and desorption on surfaces in the presence of huge electric fields.

Dislocations in covalent materials:
the puzzling complexity of cores

L. Pizzagalli

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Dislocations are extended linear defects that are usually present in most crystalline materials. Their abilities to multiply, nucleate or migrate are key attributes governing the plastic deformation in these materials. Dislocations are also largely studied because of their influence on electronic properties. Compared to other defects (like point or planar defects), a notable feature of dislocations is their long range elastic field, that has to be considered together with the short ranged core of the defect. This specificity makes it harder to describe dislocations using atomic scale simulations, in particular with first principles methods [1].

Recent advances show that in semiconductors, the dislocation core has a prominent influence on both plasticity and electronic properties. It is also increasingly acknowledged that different core configurations could be active depending on the conditions. Consequently, it is difficult to understand the influence of the dislocations and determine the relevant mechanisms.

This presentation will include two parts, two illustrative examples of the influence of dislocation cores on the properties of covalent materials. In the first one, I will focus on AlN and InN, both being important materials for opto-electronic applications. Recent first principles calculations revealed original dislocation core structures [2], highlighting the variety of possible geometries. In the second example, new results on the role of dislocation cores in the plastic deformation of covalent nanostructures will be presented. Compared to bulk, very high stresses can be attained in these systems, without fracture. I will show how these stresses completely change the traditional picture of silicon plasticity, with experiments and simulations revealing unexpected dislocation cores as vectors of plastic deformation [3-5].

[1] D. Rodney, L. Ventelon, E. Clouet, L. Pizzagalli, and F. Willaime, Acta Materialia, 124 (2017) 633-659.
[2] L. Pizzagalli, I. Belabbas, J. Kioseoglou, and J. Chen, to appear in Phys. Rev. Materials (2018).
[3] A. Merabet et al., submitted to Acta Materialia (2018).
[4] E. Maras, L. Pizzagalli, T. Ala-Nissila, H. Jónsson, Scientific Reports 7 (2017) 11966.
[5] L. Pizzagalli, S. Brochard, and J. Godet, Philos. Mag. 98 (2018) 1151-1169.

Engineering of spin defects in silicon carbide for quantum applications

G. V. Astakhov[1], C. Kasper[2], H. Kraus[3], W. Kada[4], T. Ohshima[5], D. Dyakonov[2]

1- Helmholtz-Zenrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany
2- Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg, Germany
3- NASA Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109, USA
4- Faculty of Science and Technology, Gunma University, Kiryu, Gunma 376-8515, Japan
5- National Institutes for Quantum and Radiological Science and Technology (QST), Takasaki, Gunma 370-1292, Japan

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Building quantum devices based on silicon carbide (SiC) is highly desirable, facilitated by established SiC CMOS technology. Optoelectronic SiC devices have already been demonstrated, however, the signal- mediating quantum defects are usually introduced in a semi-random manner, by bulk electron or neutron irradiation. We present the controlled generation of quantum centers in silicon carbide (SiC) by focused proton beam in a noncomplex manner without need for pre- or postirradiation treatment [1]. The generation depth and resolution can be predicted by matching the proton energy to the material's stopping power, and the amount of quantum centers at one specific sample volume is tunable from ensembles of millions to discernible single photon emitters [2]. We identify the generated centers as silicon vacancies through their characteristic magnetic resonance signatures and demonstrate that they possess highly coherent spin properties even at room temperature [3].

[1] H. Kraus et al., Nano Lett. 17 (2017) 2865.
[2] F. Fuchs et al., Nat. Commun. 6 (2015) 7578.
[3] D. Simin et al., Phys. Rev. B 95 (2017) 161201(R).

High Oxygen Doping of h-BN
for Electronic and Magnetic Properties Engineering

D. G. Kvashnin[1,2], Q. Weng[3,4], O. Cretu[4], M. Zhou[4], C. Zhang[4,6], D.-M. Tang[4], P. B. Sorokin[1,2,5], Y. Bando[4], D. Golberg[4,6]

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3- Leibniz Institute for Solid State and Materials Research, 01069, Helmholtzstraße 20, Dresden, Germany

4- National Institute of Material Science, 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan

5- Technological Institute for Superhard and Novel Carbon Materials, 142190, 7a Tsentralnaya street, Troitsk, Moscow, Russian Federation

6- Queensland University of Technology, 2 George St, Brisbane City QLD 4000, Australia

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Engineering of optical, electronic and magnetic properties of h-BN nanomaterials via oxygen doping and functionalization has extensively been studied in theory. However, it is still unclear to what extent these properties can be modulated using such methodology because of lack of significant experimental progresses and systematic theoretical investigations. Energy band gap plays the crucial role in solid state materials' optical and electronic properties. Design of artificial materials with suitable band gaps is of high priority in many fields, e.g. photovoltaics, sensors, photoluminescence etc. Introduction of oxygen atoms into the h-BN lattice provides a new practical route for its band gap and magnetic property engineering. Herein, we provide comprehensive theoretical predictions verified by solid experimental conformations that unambiguously answer this longstanding question. We report on the strong narrowing of the optical band gap in h-BN nanosheets and appearance of paramagnetism after oxygen doping and functionalization. Our systematic theoretical studies have predicted that the electronic properties of h-BN monoatomic sheets are tunable, and their band gap can be significantly narrowed through oxygen doping and/or functionalization. These findings pave the new way for hBN nanosheet optical, electronic and magnetic property engineering, and should breed brand-new applications of layered BN materials in optical, electrical, information and energy-related fields. Results were published in Advanced Materials journal in 2017. This work was supported by the Ministry of Education and Science of the Russian Federation in the framework of Increase Competitiveness Program of NUST «MISiS» (№ К2-2017-001).

Tuesday
10 July

Tuesday, 10 July 2018

09:00 - 11:20 Session 3   Chair: V. Meunier

09:00   A. Zobelli (Université Paris Sud, France)
Luminescence at defects in h-BN : excitons at stacking faults and single photon emitters

09:40   H.-P. Komsa (Aalto University, Finland)
Formation energies and defect levels of charged defects in 2D materials

10:20   M. Scardamaglia (University of Mons, Belgium)
What happens to graphene-coated copper during realistic oxidation conditions?

10:40 Coffee break

11:20 - 15:00 Session 4   Chair: P. Bøggild

11:20   K. Suenaga (AIST, Japan)
Electron Microscopy and Spectroscopy of Defects in Low-Dimensional Materials

12:00   V. Meunier (Rensselaer Polytechnic Institute, USA)
Electrons and vibrations meet defects in reduced dimensions

12:40   M. Pizzochero (EPFL, Switzerland)
Intrinsic and engineered point defects in two-dimensional 1T'-MoS$_2$

13:00 Lunch break

15:00 - 16:20 Session 5   Chair: J. Neugebauer

15:00   A. Jorio (Universidade Federal de Minas Gerais, Brazil)
Defect dimensionality in micro- and nano-Raman scattering from 2D systems

15:40   C. Jin (Zhejiang University, People's Republic of China)
Direct imaging of kinetic pathways of atomic diffusion in monolayer MoS2 by ADF-STEM

16:20   Silvan Kretschmer (Helmholtz-Zentrum Dresden-Rossendorf, Germany)
Damage mechanisms in 2D materials under electron irradiation

16:40   M. Taherinejad

17:00 - 20:00 Poster session

During the poster session there will be a get-together drink with snacks for the participants.
Location: Adriatico Guest House - Lower Level

Luminescence at defects in h-BN : excitons at stacking faults and single photon emitters

<u>Alberto Zobelli</u>, Romain Bourrellier, Sophie Meuret, Michele Amato, Steffi Woo, Odile Stéphan, Luiz Tizei, and Mathieu Kociak

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Hexagonal boron nitride (h-BN) is a promising material for optical application due to a strong exciton in the far UV and several bright and stable defect emissions. Here we investigate the spatial localization of defects lines in this rich emission spectrum by employing an original cathodoluminescence system (nano-CL) integrated within a scanning transmission electron microscope. This unique experimental setup provides full emission spectra with a resolution as low as few tens of meV associated with an electron probe size of one nanometer.

We show that several high energy emissions in h-BN are related to crystal folds leading to local changes of the layer stacking order. Complementary ab-initio calculations in the framework of Many Body Perturbation Theory (GW approximation and Bethe-Salpeter equation) confirms the role of this class of defects in changing exciton energies [1]. Middle band gap emissions present a high spatial localization (~80 nm) and a typical zero-phonon line plus phonon replica spectroscopic signature, indicating a point defect origin. By combining our nano-CL system with an Hanbury Brown and Twiss (HBT) interferometer we identify a new bright and stable single photon emitter in the far UV [2]. Finally we show how different chemical fonctionalization methods can be employed to deliberately introduce additional bright local emitting centers in h-BN.

[1] R. Bourrellier, et al. ACS Photonics 1 (2014), 857 .
[2] R. Bourrellier, et al. Nano Lett. 16 (2016), 4317.

Formation energies and defect levels of charged defects in 2D materials

H.-P. Komsa[1]

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Charged defect calculations in supercells subject to periodic boundary conditions suffer from strong and long-ranged electrostatic interactions of the localized charge with its periodic images and with the neutralizing background charge. This issue is nowadays well understood in cases where the defect is inside a bulk material, and consequently the total energies can be corrected well with *a posteriori* correction schemes. However, in order to obtain reliable results in cases where the defects are introduced to systems exhibiting inhomogeneous dielectric response, the correction schemes need to be modified accordingly.

We have introduced a computational scheme to correct for the electrostatic energy errors arising from charged defects interacting with their periodic images in systems of inhomogeneous dielectrics, such as in slab calculations or in the case of two-dimensional (2D) materials [1,2]. In my talk, I give an overview of the scheme and present results both from benchmark calculations demonstrating the validity of the scheme as well as from more realistic applications [3,4]. I discuss how the defect level positions in 2D materials depend strongly on the environment around the 2D sheet and highlight future directions and challenges.

[1] H.-P. Komsa and A. Pasquarello, Phys. Rev. Lett. 110 (2012) 095505.
[2] H.-P. Komsa, N. Berseneva, A. V. Krasheninnikov, and R. M. Nieminen, Phys. Rev. X 4 (2014) 031044.
[3] H.-P. Komsa and A. V. Krasheninnikov, Phys. Rev. B 91 (2015) 125304
[4] Y.-C. Lin, S. Li, H.-P. Komsa, L.-J. Chang, A. V. Krasheninnikov, G. Eda, K. Suenaga, Adv. Funct. Mater. 28 (2018) 1704210

What happens to graphene-coated copper during realistic oxidation conditions?

M. Scardamaglia

University of Mons - Belgium

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The recent development of near ambient pressure x-ray photoelectron spectroscopy makes accessible *in operando* investigation of many phenomena otherwise impossible, as catalytic reactions, corrosion, gas sensing. Graphene, thanks to its waterproof ability, acts as a protective layer for its supporting substrate, being a good corrosion-inhibitor for metals [1]. The prevention of metal corrosion is of extreme technological importance; therefore, the investigation of the protective action of graphene must be carefully quantified.

Within this context, we performed a spatially-resolved near-ambient-pressure XPS experiment [2] on graphene-coated copper during oxidation conditions. To understand the evolution of copper oxidation and the role of graphene, we investigated regions with bare copper, mono- and multi-layers graphene flakes. Three temperature regimes were identified:

- up to 300 °C the amorphous carbon desorbs and the Cu under graphene is still metallic, while the bare Cu regions readily oxidized;
- in a short temperature range up to 350 °C the oxygen starts to intercalate from graphene edges or defects and slightly oxidized the Cu underneath;
- for temperature higher than 350 °C the carbon is etched away and the copper under graphene changes its morphology.

With this *real-time* experiment, we clearly observed the role of graphene as a protecting layer for copper oxidation with near-ambient-pressure XPS. Up to 300 °C in O_2 atmosphere the Cu under graphene remains metallic, while at higher temperature an interesting mechanism of oxygen intercalation takes place which contributes to the oxidation of the protected copper and the etching of graphene.

[1]   M. Galbiati, A. C. Stoot, D. M. A. Mackenzie, P. Bøggild, and L. Camilli, Scientific Reports 7 (2017) 39770.
[2]   H. Sezen, M. Al-Hada, M. Amati, and L. Gregoratti, Surf. Interface Anal. (2017) DOI: 10.1002/sia.6276

Electron Microscopy and Spectroscopy of Defects in Low-Dimensional Materials

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Properties of low-dimensional materials are largely influenced by its structural imperfections, such as defects, impurities, edges or boundaries. Hence, analytical technique at single atom level is becoming crucial to fully understand the physical/chemical performance of nano-devices. In my presentation, single atom spectroscopy by means of electron energy-loss spectroscopy (EELS) will be shown to discriminate individual atoms in low-dimensional materials at their interrupted periodicities. It is emphasized here that information of the bonding/electronic states has become accessible for single atoms through the EELS fine-structure analysis [1, 2, 3] as well as the spin state [4]. Large variations of local electronic properties of 1D and 2D materials with different atomic coordinates will be investigated. Such an analysis was applied to understand catalytic behavior of Co doped MoS_2 for hydrodeoxygenation reaction [5]. Furthermore, a high-energy resolution EELS offers us possibilities to obtain local optical/vibrational properties. Some of the recent examples for such experiments on low-dimensional nanomaterials will be also presented [6-10].

[1] Y.-C. Lin et al., *Nano Letters,* **15** (2015) 7408-7413,
[2] L. Tizei et al., *Phys. Rev. Lett.*, 114 (2015) 197602,
[3] R. Senga and K. Suenaga, *Nature Communications,* (2015) 6:7943
[4] Y.-C. Lin et al., *Phys. Rev. Lett.*, **115** (2015) 206803
[5] G. Liu et al., *Nature Chem*. **9** (2017) 810
[6] J. Lin et al., *Nano Lett.*, **16**, (2016), 7198-7202,
[7] L. Tizei et al., *Phys. Rev. Lett.,* **114** (2015) 107601,
[8] R. Senga et al., *Nano Lett.,* **16**, (2016), 3661-3667
[9] Y.-C. Lin et al, *Adv. Funct. Mater.* (2017) 1704210
[10] R. Senga et al., *Nano Lett*., (2018) in press

Electrons and vibrations meet defects in reduced dimensions

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The Oxford dictionary defines the word "defect" as "*a shortcoming, an imperfection, or a lack*". The Latin etymology of the word is more instructive as it establishes that "defect" originates from *de-* (expressing reversal) + *facere* 'do'. Accordingly, in solid-state physics, a defect would be features that "undo" the existing order, especially by interrupting the perfect atomic arrangement of a crystal lattice. Thus, in this sense, a "defect" is neither a "lack" nor a "shortcoming", but rather a feature that can open up opportunities to induce new physical properties that are absent in the otherwise perfect system.

In this talk, I will provide a number of examples where defects are responsible for the emergence of fascinating properties in reduced dimensionality systems. Using the etymological definition as a guiding theme, I will focus on two types of defects: point defects (e.g., vacancy or substitutional) and extended defects (e.g., interface between two distinct ordered lattices). The examples will start from experimental evidence of defects, and their signature in characterization techniques ranging from scanning tunneling microscopy (STM) and spectroscopy (STS), Raman, and electron microscopy (TEM). I will then show how first-principles modeling provides a unique lens to understand the microscopic origin of the emerging phenomena caused by the presence of defects.

Specifically, I will first show how vacancy [1], rotational [2] and substitutional [3] defects can be controllably induced in transition metal dichalcogenides by an external stimulus and how they affect the materials' electronic and vibrational properties in a predictive, quantitative manner. The second part of my presentation will focus on carbon materials. I will describe situations where defect-free materials can be assembled and how deviations from perfection lead to the development of interfaces to create "quantum dots by-design" [4-5], atomically precise heterostructures [6], and even topologically protected interface states. [7]

Finally, my presentation will discuss how the promise of materials stochasticity can be harnessed to boost functionality and our understanding of electronic processes at the nanoscale [8], where, in general the presence of defects constitutes an opportunity rather than a curse.

References:

[1] William M Parkin, Adrian Balan, Liangbo Liang, Paul Masih Das, Michael Lamparski, Carl H Naylor, Julio A Rodríguez-Manzo, AT Charlie Johnson, Vincent Meunier, and Marija Drndić, ACS Nano 10 (2016), 4134.
[2] AC Yoshimura, M Lamparski, N Kharche, and V Meunier, Nanoscale 10 (2018), 2388
[3] AC Yoshimura and V Meunier, in press (2018).
[4] Chuanxu Ma, Liangbo Liang, Zhongcan Xiao, Alexander A Puretzky, Kunlun Hong, Wenchang Lu, Vincent Meunier, Jerzy Bernholc, and An-Ping Li, Nanoletters, 17 (2017), 6241
[5] Shiyong Wang, Neerav Kharche, Eduardo Costa Girão, Xinliang Feng, Klaus Müllen, Vincent Meunier, Roman Fasel, and Pascal Ruffieux, Nanoletters 17 (2017), 4277
[6] Jinming Cai, Carlo A Pignedoli, Leopold Talirz, Pascal Ruffieux, Hajo Söde, Liangbo Liang, Vincent Meunier, Reinhard Berger, Rongjin Li, Xinliang Feng, Klaus Müllen, and Roman Fasel, Nature Nanotechnology 9 (2014) 896.
[7] O. Gröning et al, in press (2018)
[8] Robert Hull, Pawel Keblinski, Dan Lewis, Antoinette Maniatty, Vincent Meunier, Assad A Oberai, Catalin R Picu, Johnson Samuel, Mark S Shephard, Minoru Tomozawa, Deepak Vashishth, and Shengbai Zhang, Applied Physics Reviews 5 (2018), 011302.

Intrinsic and engineered point defects in two-dimensional $1T'$-MoS$_2$

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Monolayer group VI transition metal dichalcogenides (TMDs) exist in either the semiconducting $2H$ phase or practically semimetallic $1T'$ phase. While the stable $2H$ phase has been extensively investigated due to prospective technological applications in electronics and optoelectronics, the metastable $1T'$ polymorph has appeared in the spotlight only very recently, largely due to its topological properties. Aim of this talk is to provide an overview on the formation of point defects in $1T'$-MoS$_2$ — a prototypical $1T'$-TMD — within two experimentally-relevant situations, namely under thermodynamic equilibrium and under electron beam irradiation.

Based on first-principles calculations, firstly I will address the thermodynamic stability of simple point defects, exploring several configurations of vacancy, adatom and antisite defects in sulfur-rich and molybdenum-rich conditions [1]. All considered defects present lower formation energies in the $1T'$ phase compared to the $2H$ phase, suggesting that the $1T'$ polymorph is expected to be more susceptible to lattice imperfections. Next, the response of $1T'$-MoS$_2$ to the electron irradiation will be presented [2]. The range of electron beam energies needed to carry out sample imaging without inducing any radiation damages in the lattice and some guidelines for the controlled introduction of defects in the transmission electron microscope are discussed in the light of our molecular dynamics simulations.

Throughout the talk, I will draw comparisons between local disorder in the $1T'$ polymorph and the well-studied $2H$ phase in order to portray a complete picture of the role of defects in the different crystalline phases of two-dimensional transition metal dichalcogenides.

[1] M. Pizzochero and O. V. Yazyev, Phys. Rev. B. 96, 245402 (2017)
[2] M. Pizzochero and O. V. Yazyev, 2D Mater, in press (2018)

Defect dimensionality in the micro- and the nano-Raman scattering from two-dimensional systems

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Raman spectroscopy has been largely used to quantify defects in graphene and other two-dimensional (2D) materials. Here we discuss how Raman spectroscopy can be used to disentangle the information from one-dimensional (1D) and zero dimensional (0D) defects in 2D materials (see Figure 1) [1].

From the dimensionality standpoint, defects in two-dimensional systems can be either one- (1D) or zero-dimensional (0D). In graphene, both types of defects produce changes in the Raman spectrum, and identifying separately the contribution from each defect-type is a challenge. Here we show that a diagram can be built for disentangling contributions of point-like and line-like defects to the Raman spectra of graphene-related materials embracing, from the topology point of view, all possible structures from perfect to fully disordered sp^2 bonded carbons. The procedure has been parameterized for graphene using well-controlled reference materials with only 0D [2] or 1D defects [3]. We then discuss the limitations and apply our new methodology to analyze the structure of two-dimensional nanocarbons generated from renewable gas, used to produce inks and conducting coatings.

We develop our analysis for the case of tip-enhanced Raman spectroscopy (TERS), where we achieve characterization with nanometer resolution. We compare a massive amount of data obtained with micro and nano-Raman characterization for a comparative analysis [4].

[1] LG Cançado, MG da Silva, EH Martins Ferreira, F Hof, K Kampioti, K Huang, A Pénicaud, CA Achete, RB Capaz and A Jorio, 2D Mater. 4 (2017) 025039

[2] MM Lucchese, F Stavale, EH Martins Ferreira, C Vilani, MVO Moutinho, RB Capaz, CA Achete, A Jorio, Carbon 48 (2010) 1592–1597

[3] J Ribeiro-Soares, ME Oliveros, C Garin, MV David, LGP Martins, CA Almeida, EH Martins-Ferreira, K Takai, T Enoki, R Magalhaes-Paniago, A Malachias, A Jorio, BS Archanjo, CA Achete, LG Cançado. Carbon 95 (2015) 646-652

[4] Cassiano Rabelo. Umpublished.

Direct imaging of kinetic pathways of atomic diffusion in monolayer MoS₂ by ADF-STEM

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Direct observation of atomic migration both on and below surfaces is a long-standing but important challenge in materials science as diffusion is one of the most elementary processes essential to many vital material behaviors. Probing the kinetic pathways, including metastable or even transition states involved down to atomic scale, holds the key to the underlying physical mechanisms. Here, we applied aberration corrected transmission electron microscopy (TEM) to demonstrate direct atomic-scale imaging and quasi-real-time tracking of diffusion of Mo adatoms and vacancies in monolayer MoS₂, an important two-dimensional transition metal dichalcogenide (TMD) system. Preferred kinetic pathways and the migration potential-energy landscape are determined experimentally and confirmed theoretically. The resulting three-dimensional knowledge of the atomic configuration evolution reveals the different microscopic mechanisms responsible for the contrasting intrinsic diffusion rates for Mo adatoms and vacancies. The new insight will benefit our understanding of material processes such as phase transformation and heterogeneous catalysis.

Adsorption and kinetic pathway of Mo adatom on monolayer MoS₂
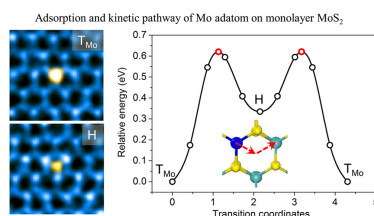
[1] J. Kotakoski, C. Mangler, J. C. Meyer, Nat. Commun. 5 (2014) 3991.
[2] J. H. Hong et al., Nano Lett. 17 (2017) 3383.
[3] DFT calculations were done by Prof. Wei Ji's group from Department of Physics, Renmin University of China. The authors acknowledge financial support from NSFC, MOST, and the access to microscope facilities kindly provided by the Center of Electron Microscopy of Zhejiang University.

Damage mechanisms in 2D materials under electron irradiation

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As the influence of defects on material properties heavily depends on the dimensionality, understanding defect production mechanisms in detail plays a major role for two-dimensional (2D) materials. The defect production under irradiation e.g. in the transmission electron microscope (TEM) can be subdivided into three mechanisms, namely knock-on damage, ionization damage and chemical etching. Surprisingly, as shown for transition metal dichalcogenides, in TEM defects are produced far below the knock-on threshold [1]. Here we investigate ionization and excitation damage mechanisms for Graphene, MoS_2 and hexagonal BN using first-principles simulation techniques.

[1]   Y.Lin, T.Björkman, H.Komsa et al. Nature Communications 6, 6736, 2015

Strong Levinson Theorem in Periodic Systems

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We study the relationship between the phase shift of scattering states and the bound states localized on impurity or defects in periodic systems. The presence of defects in a quantum system leads to emergence of eigenstates in the energy ranges inaccessible to the unperturbed system. These new eigenstates are as a matter of fact the scattering states which are pulled out of the allowed energy spectrum of the unperturbed system by the perturbation and transformed into bound states localized around the defect. The remaining scattering states undergo a phase shift in response to the perturbing potential. The relationship between this phase shift of scattering states and the number of bound states created by the defect is known as Levinson theorem [1] and has been proved in both nonrelativistic and relativistic regimes. In 1966 Callaway [2] derived a form of the Levinson theorem for the scattering of an excitation in a solid by a potential of finite range, which shows the relationship between the phase shift at the upper $\delta(E_n^u)$ and lower $\delta(E_n^l)$ edges energy band n and the spectral deficiency of that band N_n

$$\delta(E_n^l) - \delta(E_n^u) = \pi N_n .\tag{1}$$

We derive a strong from of Levinson theorem in periodic systems for the phase shift at each band edge $\delta_l(E_n^s)$, where s specifies the upper or lower edge of energy band n, and l is the quantum number of scattering state. We show that the phase shift at each band edge is quantized and proportional to the number of states of the same quantum number which are transformed into bound states from that edge

$$\delta_l(E_n^s) = \pi N_{l,n}^s .\tag{2}$$

By adiabatic variation of scattering potential strength some of the bound states may shift toward the edge of a neighboring band and eventually join it. Naturally, a bound state crossing into an energy band contributes to the phase shift of the scattering states at the band edge by $-\pi$.

[1] Levinson N 1949 Kgl. Danske Videnskab. Selskab Mat.-fys. Medd. 25 No. 9.
[2] J. Callaway, Phys. Rev. **154** (1967) 515.

Wednesday
11 July

09:00 - 11:20 Session 6   Chair: J. Kotakoski

09:00   M. Nastasi (University of Nebraska at Lincoln, USA)
             Ion-Solid Interactions and Defect Formation

09:40   A. Vantomme (KU Leuven, Belgium)
             Implantation-induced defects and lattice site of impurities in semiconductors

10:20   M. Anđelković (Universiteit Antwerpen, Belgium)
             Effects of disorder and resonant scattering in twisted bilayer graphene

10:40 Coffee break

11:20 - 14:00 Session 7   Chair: H. –P. Komsa

11:20   J. Kotakoski (University of Vienna, Austria)
             On 2D materials and their defects under electron irradiation

12:00   P. Bøggild (DTU Nanotech, Denmark)
             Graphene at the edge of perfection

12:40   R. Niyazov (National Research Center «Kurchatov Institute», Russian Federation)
             Aharonov-Bohm interferometer on helical edge states: Coherent enhancement of scattering off magnetic impurity

13:00 Lunch break

14:00 - 22:00 Excursion and dinner

Ion-Irradiation-Induced Defects in Solids

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This talk will focus on ion irradiation and defect formation in solids. Sources of ion irradiation will be discussed. We will explore the concept of ion stopping in materials and how energy deposition into the nuclear system of the solid result in the production of atomic displacements and defect formation. The use of microstructure to control defect retention in materials will be discussed. Examples will be given using nanostructured materials and amorphous materials.

Implantation-induced defects and lattice site of impurities in semiconductors

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In order to (locally) tailor the functional properties of semiconductors, be it electric, optic, or magnetic, one typically relies on ion implantation. Indeed, by selecting a suitable combination of ion energy and fluence, excellent control is obtained of the dopant depth profile as well as its concentration. Moreover, the mass separation used in ion implantation assures an isotopically pure beam, hence circumventing any potential impurity issue.

However, the abundant atomic collisions taking place during the slowing down of the implanted ions, result in a large defect concentration, in particular vacancy-interstitial pairs. Although a large fraction of these defects recombines quasi-instantly, an appreciable amount typically survives, thus impacting the functional properties of the semiconductor. Moreover, these properties are also strongly dependent on the exact lattice sites occupied by the dopant – the latter being directly affected by remaining defects in its surrounding. Therefore, detailed knowledge on defect generation during the implantation process, defect recovery and lattice site are indispensable. Amongst others, channeling of energetic charged particles is ideally suited to obtain this information with sub-Å precision. In this talk, we give an overview of recent lattice location studies for impurities and dopants in ZnO and GaN, as representative wide-gap semiconductors.

Although the main occupied site, for a given impurity-host combination, can often be predicted based on chemical similarities between impurity and host elements, such expectations fail in many cases. Furthermore, minority sites (in case of multiple-site occupancy) are even more difficult to predict, detect and identify. These experiments are based on an exotic variety of the channeling technique, i.e. emission channeling (EC), using radioactive isotopes produced at the ISOLDE facility at CERN. EC makes use of the charged particles emitted by a radioactive isotope upon decay. The screened Coulomb potential of atomic rows and planes determines the anisotropic scattering of the particles emitted isotropically during the radioactive decay. Along low-index directions of single crystals and epitaxial films, this anisotropic scattering results in well defined channeling or blocking effects. Because these effects strongly depend on the initial position of the emitted particles, they result in emission patterns which are characteristic of the lattice site(s) occupied by the probe atoms.

In this talk, we present some particular cases that illustrate the strengths of emission channeling when studying systems exhibiting multiple-site occupancy. The selected systems comprise transition metals in ZnO and GaN [1, 2 ,3, 4], Mg in AlN [5] and in GaN [6], and rare earth ions in GaN and AlN [7, 8, 9]. Special attention will be devoted to the role of implanted fluence, the implantation temperature, the annealing temperature, as well as the doping character of the semiconductor and the role of implantation damage.

[1] L.M.C. Pereira *et al.*, Phys. Rev. B84, 125204 (2011).
[2] L.M.C. Pereira *et al.*, Phys. Rev. B86, 195202 (2012).
[3] U. Wahl *et al.*, Appl. Phys. Lett. 78, 3217 (2001).
[4] L.M.C. Pereira *et al.*, Appl. Phys. Lett. 103, 091905 (2013).
[5] L.M. Amorim *et al.*, Appl. Phys. Lett. 103, 262102 (2013).
[6] U. Wahl *et al.*, Phys. Rev. Lett. 118 (2017) 095501.
[7] A. Vantomme et al., Topics in Appl. Phys. 124, Ch. 3, 55-98 (2010).
[8] B. De Vries et al., Appl. Phys. Lett. 84, 4304 (2004).
[9] B. De Vries et al., Appl. Phys. Lett. 103, 172108 (2013)

Effects of disorder and resonant scattering in twisted bilayer graphene

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Twisting of bilayer graphene opened up a playground for engineering devices of arbitrary functionality, changing the behaviour from metallic to semiconducting [1, 2], or even superconductive [3]. Such richness of properties is a consequence of the coupling between graphene layers, which strongly depends on the twisting angle. More importantly, recent experiments have proven the possibility to finely tune the rotation angle with an accuracy even bellow a half of degree. Nevertheless, although the fabrication methods have been improved significantly since the discovery of graphene, procedures of changing the orientation of graphene flakes necessarily will induce defects in the sample.

In this study, we examine the atomistic disorder effects in twisted bilayer graphene within a real-space tight-binding methodology. The spectral properties such as density of states, global and local and DC conductivity in a linear response Kubo formalism are calculated following an expansion in terms of Chebyshev polynomials [4]. Large size of computational system that we consider, obtainable due to the two-dimensional nature of the problem, and the numerical efficiency of the method, give us the freedom to easily model different disorder types, changing both their concentration and strength, while being in regimes that reflect the experimental samples. Therefore, we are able to easily examine effect of different disorder, starting from vacancies that are strong short-range scatterers [5], to disorder with long-range distribution such as charge puddles. For different twist angle, we show the effects of disorder with different width, and discuss on the resonant scattering that will change the coupling between the two layers, hence induce the interlayer scattering, and deteriorate the transport properties.

[1] K. Kim, A. DaSilva, S. Huang, B. Fallahazad, S. Larentis, T. Taniguchi, K. Watanabe, B. J. LeRoy, A. H. MacDonald and E. Tutuc, Proc. Natl. Acad. Sci. **114**, 3364 (2017).
[2] Y. Cao, V. Fatemi, A. Demir, S. Fang, S. L. Tomarken, J. Y. Luo, J. D. Sanchez-Yamagishi, K. Watanabe, T. Taniguchi, E. Kaxiras, R. C. Ashoori, and P. Jarillo-Herrero, Nature **556**, 80–84 (2018).
[3] Y. Cao, V. Fatemi, S. Fang, K. Watanabe, T. Taniguchi, E. Kaxiras and P. Jarillo-Herrero, Nature **556**, 43–50 (2018).
[4] J. H. García, L. Covaci and T. G. Rappoport, Phys. Rev. Lett. **114**, 116602 (2015).
[5] M. Anđelković, L. Covaci and F. M. Peeters, Phys. Rev. Materials **2**, 034004 (2018).

On 2D materials and their defects under electron irradiation

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The discovery of mono-layer graphene more than a decade ago occurred at a fortunate time in terms of transmission electron microscopy (TEM)—aberration-corrected TEM instruments that allowed imaging of materials at low acceleration voltages (at and below 80 kV) became available approximately at the same time.

On the one hand, as a one-atom thick membrane of carbon atoms, graphene serves as the ideal material for TEM, which requires thin samples and provides projected images of the atomic structure. On the other hand, due to the light mass of the carbon atoms, elastic scattering of electrons accelerated at close to 80 kV can transfer them enough momentum to enable atomic-scale dynamics. This combination allowed for the first time the atomic-resolution study of the so-called knock-on damage [1,2] as well as structural modification of graphene [3], its defects [4,5], edges [6] and even impurity atoms [7-10]. With the 1-Å beam size of modern scanning TEM (STEM) devices, these effects can even be localized down to individual atoms.

In addition to elastic scattering, due to ionization also inelastic scattering of electrons can lead to structural changes in a material. While this is not an issue for conducting materials such as graphene where ionization is quenched at a time scale faster than atomic dynamics, it is an issue for semiconducting and insulating materials. Moreover, the inelastic scattering cross section increases for lowering acceleration voltages and increasing atomic numbers. This makes it a significant contributor to the observed structural changes in most inorganic 2D materials, such as hexagonal boron nitride [11], MoS_2 [12] and $MoTe_2$ [13], but can be suppressed by graphene encapsulation. Encapsulation also allows creating novel molecular arrangements, such as mono-layer fullerene crystals [14] and their imaging at the atomic resolution.

Finally, in non-ideal vacuum conditions electron irradiation can also lead to the activation of chemical processes due to cracking of molecules in the residual vacuum near the sample surface. While the knock-on and ionization damage can be controlled by tuning the acceleration voltage and encapsulation, controlling chemical processes requires a ultra-high vacuum microscope column and control over the residual gas pressure and composition.

In this presentation, I aim to demonstrate that the possibility for controlling all of the beam-induced structure-altering mechanism together with the atomic-size probe of modern STEM devices is establishing modern STEM not just an imaging technique, but also a way to engineer materials down to individual atoms.

[1] J. C. Meyer et al., Phys. Rev. Lett. 108, 196102 (2012)
[2] T. Susi et al., Nat. Commun. 7, 13040 (2016)
[3] J. Kotakoski et al., Phys. Rev. Lett. 106, 105505 (2011)
[4] J. Kotakoski et al., Nat. Commun. 5, 4991 (2014)
[5] S. Kurasch et al., Nano Lett., 12, 3168-3173 (2012)
[6] J. Kotakoski et al., ACS Nano 6, 671-676 (2012)
[7] T. Susi et al., ACS Nano 6, 8837-8846 (2012)
[8] T. Susi et al., Phys. Rev. Lett. 113, 115501 (2014)
[9] T. Susi et al., 2D Mater. 4, 042004 (2017)
[10] T. Susi et al., Sci. Rep. 7, 4399 (2017)
[11] J. Kotakoski et al., Phys. Rev. B 82, 113404 (2010)
[12] H.-P. Komsa et al., Phys. Rev. Lett., 109, 035503 (2012)
[13] K. Elibol et al., Chem. Mater. 30, 1230-1238 (2018)
[14] R. Mirzayev et al., Sci. Adv. 3, e1700176 (2017)

Graphene at the edge of perfection

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Defects and disorder of graphene edges has held back development of graphene nanoelectronics for more than a decade. While lithographic patterning of graphene on the scale of 10 nm has been demonstrated both with top-down (electron-beam lithography) and bottom-up methods (i.e. block copolymer lithography), the predicted tunable bandgap and high-mobility waveguide-like behavior has not. I will show some examples of how edge disorder can be tamed to a point where genuinely new transport behavior emerges, including recently observed suppression of the quantum Hall effect in edge-polished nano-constrictions[1], true bandgaps in ultradense antidot lattices etched through encapsulated graphene[2,3] and ferroelectric switching of polar molecules at the edge of graphene[4]. I will also touch upon the options for creating disorder free edges in graphene by etching processes [5].

[1] J. Caridad et al, Nature Communications, Nature Comm., 9 (2018) 659
[2] B. S. Jessen, L. Gammelgaard et al, unpublished.
[3] F. Pizzocchero, L. Gammelgaard, B. S. Jessen et al, Nature Comm., 7 (2016) 11894
[4] J. Caridad et al, submitted.
[5] T. J. Booth et al, Nano Lett., 11 (2011) 2689

Aharonov-Bohm interferometer on helical edge states: Coherent enhancement of scattering off magnetic impurity

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The wave nature of electrons is manifested in a quantum-coherent phenomenon - interference. This phenomenon is the foundation of devices, named interferometers, which is used for high-sensitivity measurement of the magnetic field, electron spin control and for quantum computation. We discuss the transport of electrons through the Aharonov-Bohm interferometer [1] which is created on the helical edge states connected to metallic leads. The dependence of the electron transport on the magnetic flux piercing the area encompassed by edge states is studied. We consider the case of relatively high temperatures as compared to the distance between the energy levels of the system [2].

It is shown [3] that the tunnel conductance of the interferometer does not depend on the magnetic flux in the ballistic case. Nevertheless, it has a sharp resonance as a function of the magnetic flux in the presence of a magnetic impurity. This resonance behavior can be related to the coherent enhancement of forward and back scattering by a magnetic impurity - a very similar effect to the phenomenon of weak localization.

[1] A. G. Aronov and Y. V. Sharvin, Rev. Mod. Phys. 59 (1987) 755.
[2] A.P. Dmitriev, I.V. Gornyi, V.Y. Kachorovskii, D.G. Polyakov, Phys. Rev. Lett., 105 (2010) 036402.
[3] R.A. Niyazov, D.N. Aristov, V.Yu. Kachorovskii, arXiv:1804.01115.

Thursday
12 July

09:00 - 11:20 Session 8   Chair: G. –D. Lee

09:00   M. Schleberger (Duisburg-Essen University, Germany)
Ion Irradiation Induced Defects in 2D Materials

09:40   D. Golberg (Queensland University of Technology, Australia)
In-situ TEM Methods for Analysis of Nanomaterial Defects/Properties Relationships

10:20   C. Hofer (University of Vienna, Austria)
Revealing the 3D Structure of Graphene Defects

10:40 Coffee break

11:20 - 15:00 Session 9   Chair: M. Schleberger

11:20   G. D. Lee (Seoul National University, South Korea)
Cooperative Research of Simulations and Experiments for Structural Change of Carbon Linear Chains and MoS_2

12:00   M. Edmonds (University of Bath, United Kingdom)
Defects in WSe_2 investigated by Quasi-Particle Interference mapping and STM/STS

12:20   J. Yu (Seoul National University, South Korea)
Half-metallic ferromagnetism induced by Sn-doping in $SrRuO_3$ perovskite oxides

12:40   J. Strand (University College London, United Kingdom)
DFT study on Intrinsic Defects in h-BN

13:00 Lunch break

15:00 - 17:00 Session 10   Chair: D. Golberg

15:00   U. Bangert (University of Limerick, Ireland)
Electron-Microscopy and -Spectroscopy of Defects in 2-D Materials

15:40   M. Tripathi (University of Vienna, Austria)
Ion and electron beam modification of graphene

16:00   A. Novikav (Institute of Physics NAS, Belarus)
Spectral properties of radiation-induced near-cluster color centers in LiF, NaF and MgF_2 nanocrystals

16:20 Coffee break

17:00 - 18:20 Session 11   Chair: K. Kaasbjerg

17:00   D. Efremov (IFW, Dresden, Germany)
Disorder in multi-band superconductors

17:40   V. Carnevali (Universita' degli Studi di Trieste, Italy)
Vacancy defects with trapped adatoms in epitaxial graphene on Ni(111)

18:00   E. Kogan (Bar-Ilan University, Israel)
To have (Kondo Effect) and have not: Renormalization and scaling

18:20   D. Fil (Institute for Single Crystals NASU, Ukraine)
First-principles study of defect complexes in Ti-doped sapphire

Ion Irradiation Induced Defects in 2D Materials

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Two-dimensional (2D) materials attract the attention of scientist and engineers alike. In their pristine form 2D materials exhibit often superior and sometimes even unique properties enabling both, the investigation of novel physical phenomena as well as the implementation of innovative devices, applications, and technologies. An important issue in this context are defects which will always be present in any given 2D material and may affect the material properties in various ways. From material science it is well known that defects are not necessarily detrimental, fabricated in a controlled way they may very well be advantageous or may even represent the key to functionality, e.g. chemically active sites for catalysis [1] or well-defined pores for membrane-based applications such as ultrafiltration [2]. For 3D materials a whole tool-box for the controlled fabrication of such defects already exist, and ion irradiation represents an important and well-established tool from this box. For 2D materials this tool has proven to be equally efficient (see e.g. [3]) but it needs to be adapted and optimized because different creation mechanisms have to be taken into account. In this talk I will present several examples of defect creation in various 2D materials by ion irradiation with a focus on individual impact of energetic ions, including highly charged ions [4] and swift heavy ions [5,6].

[1] G. Li et al., J. Am. Chem. Soc. 138 (2016) 16632
[2] O'Hern et al., ACS Nano 6 (2016) 10130
[3] Z. Li et al., Applied Physics Reviews, 4 (2017) 011103
[4] J. Hopster et al., 2D Materials 1 (2014) 1011011
[5] L. Madauß et al., 2D Materials, 4 (2017) 015034
[6] L. Madauß et al., Nanoscale 9 (2017) 10487

In situ TEM Methods for Analysis of Nanomaterial Defects/Properties Relationships

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Understanding mechanical, electrical, thermal, thermoelectric, optical, optoelectronic and photovoltaic properties of a nanomaterial, in particular, on the individual nanostructure level, is of key importance as far as its smart integration into modern sustainable technologies is concerned.

However, in the vast majority of cases, such property measurements have been performed by means of instruments with no direct access to the materials' atomic structure, its crystallography, spatially-resolved chemistry and existing point and/or linear structural defects. This fact largely limits the relevance of the collected data, because all particular structural features of an object prior, during and after its testing are typically hidden. Therefore, the acquired results can hardly be linked to particular nanomaterials' morphology, atomic structure, and defect networks. Thus, a wide scatter in the reported data has been commonly observed between various samples and research groups. Till now this drawback has greatly confused practical engineers and technologists and led to many uncertainties in regards to nanomaterials' industrial potentials and practical applications.

In this contribution I demonstrate the full usefulness of utilized by my groups *in situ* high resolution transmission electron microscopy (HRTEM) probing techniques for diverse property analyses of many advanced materials, *e.g.* individual inorganic nanotubes, graphene-like nanosheets, nanowires and nanoparticles, and unambiguous analysis of their atomic/defect structure-property relashioships [1-14].

Elasticity, plasticity, fracture strength and toughness, electrical conductance, thermal gradients, photocurrents, photovoltages and spatially-resolved cathodoluminescence were accurately measured inside HRTEM, while employing piezo-driven nanomanipulators and/or optical fibers inserted into the microscope column.

[1] D. Golberg et al. Nano Lett. 7 (2007) 2146.
[2] D. Golberg et al. Adv. Mater. 24 (2012) 177.
[3] M.S. Wang, D. Golberg et al. Adv. Mater. 22 (2010) 4071.
[4] X.L. Wei, D. Golberg et al. Adv. Mater. 22 (2010) 4895.
[5] D.M. Tang, D. Golberg D. et al. Nano Lett. 12 (2012) 1898.
[6] X.L. Wei, D. Golberg et al. Nano Lett. 15 (2015) 689.
[7] P. Costa, D. Golberg et al. Nature Commun. 2 (2011) 4121.
[8] D.M. Tang, D. Golberg et al. Nano Lett. 15 (2015) 4922.
[9] D.M. Tang, D. Golberg et al. Nature Commun. 5 (2014) 3631.
[10] C. Zhang, D. Golberg et al. Appl. Phys. Lett. 107 (2015) 091103.
[11] K.E. Moore, O. Cretu, M. Mitome, D. Golberg, Carbon 107 (2016) 225.
[12] C. Zhang, D. Golberg et al. Nano Lett. 16 (2016) 2054.
[13] M.S. Wang, D. Golberg et al. ACS Nano 11 (2017) 10575.
[14] J. Fernando, C. Zhang, K. Firestein, D. Golberg, Small 13 (2018) 1701564.

Revealing the 3D Structure of Graphene Defects

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We demonstrate insights into the three-dimensional structure of defects in graphene, in particular grain boundaries and silicon dopants, obtained via a new approach from two transmission electron microscopy images recorded at different angles. The structure is obtained through an optimization process where both the atomic positions as well as the simulated imaging parameters are iteratively changed until the best possible match to the experimental images is found. We first demonstrate that this method works using an embedded defect in graphene that allows direct comparison to the computationally predicted three-dimensional shape. We then applied the method to a set of grain boundary structures with misorientation angles nearly spanning the whole available range (2.6-29.8°). The measured height variations at the boundaries reveal a strong correlation with the misorientation angle with lower angles resulting in stronger corrugation and larger kink angles. We also used our technique to reveal the 3D structure of silicon substitutes, silicon trimers and silicon tetramers. Because electrons also transfers momentum to our object of interest, electron beam induced dynamics are also visualized via our approach. Our results allow for the first time a direct comparison with theoretical predictions for the corrugation at grain boundaries and silicon dopants.[1]

[1] Hofer et. al, submitted (2018).

Cooperative Research of Simulations and Experiments for Structural Change of Carbon Linear Chains and MoS2

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The structural changes in low dimensional materials has been a long time subject of intensive investigation because the structural and electronic properties are determined by the structure. In order to study the structural changes, many state-of-art observation techniques such as transmission electron microscopy (TEM) and scanning tunneling microscopy techniques have been developed and utilized. However, since the process of structural change is finished in a very short time, it is very difficult to clarify the process and the origin of structural changes even within the state-of-the-art microscopy methods. On the other hands, various simulation methods have been developed to study and predict the property of materials. Among those methods, the density functional theory (DFT) calculation method is widely used due to the accuracy and predictability. The tight-binding molecular dynamics (TBMD) simulation method is also attempted to study the dynamics in materials. In the cooperative research of DFT calculation, TBMD simulation method, and TEM experiment, I studied successfully defects and dopants in 2D materials [1-4] as well as structural changes in nanomaterials [5,6]. In this talk, the recent results on the structural changes of carbon double linear chains and the phase transition of MoS2 will be introduced. Under the electron irradiation, the carbon double linear chains are found in the graphene constriction. In the short double linear chain, the reversible aromatic ring cyclization, so-called Bergman cyclization is observed. Our TBMD simulation is exploited to explain the structural changes in carbon double linear chain. It is also found the phase transition in MoS2 patch is induced by gas molecule and it improves greatly the catalyst effect. The origin of the phase transition is explained in atomic scale by using DFT calculation method.

[1] K. He et al., Nature Communications 5:3040 (2014).
[2] A. W. Robertson et al., Nano Letters, 15 5950 (2015)
[3] S. Wang et al., ACS Nano 10, 5419 (2016)
[4] A. W. Robertson et al., ACS Nano 10, 10227 (2016)
[5] Dae-Hyun Nam et al. Advanced Materials 29, 1702958 (2017)
[6] Min Sup Choi et al. Advanced Materials 29, 1703568 (2017)

Defects in WSe2 investigated by Quasi-Particle Interference mapping and STM/STS

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Defects in transition metal dichalcogenides (TMDs) are local atomic modifications which can affect the electronic and magnetic properties of the material. Here we focus on WSe2 which is one of the semiconducting TMDs and has great potential in both spintronics and valleytronics. We studied natural defects in WSe2 crystals and monolayers by scanning tunnelling microscopy and spectroscopy (STM/STS), coupled with quasiparticle interference (QPI) mapping, at 4K and 77K. Among a large variety of defect configurations, we identified a few that based on QPI appear to support spin-flip processes. We have also studied monolayers of WSe2 on atomically flat metallic surfaces and used QPI to characterise their interaction and defect behaviour.

Half-metallic ferromagnetism induced by Sn-doping in SrRuO₃ perovskite oxides: A first-principles prediction

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Half-metallic ferromagnets (HMFs) have attracted considerable interest as a new class of materials with potential applications for its possible memory and spintronic device applications.[1] An ideal half-metal has only one spin channel for conduction, that is, metallic behavior in one spin channel but an insulating gap in the other spin channel. However, while many different HMFs have been suggested, its fabrication has been challenging. Here we propose Sn-doped SrRuO₃ perovskite oxides as a candidate material for HMF. SrRuO₃ is one of the most frequently used oxide electrode materials.[2] It has high chemical stability and good thermal properties, which are advantageous for integration with other oxide materials into heterostructures. Because of the similar ionic sizes of Ru^{4+} and Sn^{4+} ions, the substitution of Ru by Sn atoms in SrRuO3 is quite feasible. At the endpoints of $SrRu_{1-x}Sn_xO_3$, SrRuO₃ is a ferromagnetic metal while SrSnO₃ is a large gap semiconductor with the optical gap of around 4 eV. Since the band gap of SrSnO₃ is larger than the Ru t_{2g} bandwidth of less than 3 eV in SrRuO₃, the Sn atom at the Ru site is expected to block the hopping of Ru d electrons effectively. We investigated the electronic and magnetic properties of $SrRu_{1-x}Sn_xO_3$ by carrying out density-functional-theory calculations to show that a half-metallic ferromagnetic ground state emerges for the Sn doping of $x \geq 0.5$.[3] To examine the effect of on-site Coulomb interactions for the Ru d orbitals, which was suggested to enhance the half-metallicity in SrRuO₃, we employed both the local spin-density approximation (LSDA) as well as the LSDA + U method. For all the possible configurations of Sn doping for x = 1/8, 1/4, 1/2, 5/8, 3/4, and 7/8 within the 2 × 2 × 2 unit cell, we monitor the Ru t_{2g} bandwidth as well as the valence band maximum in the majority-spin channel and demonstrate that the Ru d electron hopping is blocked by the Sn-substituted sites so that the Ru t_{2g} bandwidth becomes reduced as the doping x increases. For x < 0.5, the valence band maximum still touches the Fermi level so that $SrRu_{1-x}Sn_xO_3$ remains as a usual ferromagnetic metal. A further reduction of the Ru t_{2g} bandwidth for the range of 0.5 < x < 0.7 turns it into a half-metallic ferromagnet. As for x > 0.7, the Ru t_{2g} bandwidth gets so narrow that even a small on-site Coulomb interaction, e.g., U_{eff} = 1.0 eV induces a band-gap, which indeed corresponds to a gap of the Ru impurity bands in the SrSnO₃ oxide semiconductor.

[1] W.E. Pickett, J.S. Moodera, Phys. Today 54 (5) (2001) 39–44.
[2] M. Stengel, N.A. Spaldin, Nature 443 (2006) 679.
[3] Namwook Kim, Rokyeon Kim, Jaejun Yu, Journal of Magnetism and Magnetic Materials 460 (2018) 54.

DFT study on Intrinsic Defects in hBN

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Boron nitride is a promising candidate as a dielectric layer in 2D-material based devices [1]. Bulk hexagonal boron nitride (hBN) is isostructural to graphite, forming a layered honeycomb structure where boron and nitrogen atoms are held together by strong sp^2 bonds, giving hBN excellent mechanical strength and chemical stability [2,3]. Likewise, single layer hBN is also isostructural with graphene. Unlike graphene, however, single layer hBN is an insulator with a nonzero band gap between 5 and 6 eV [4].

In devices, semiconductor function is affected by the presence of intrinsic defects. For example, it is known that oxygen vacancies in semiconducting oxides (SiO_2, HfO_2) are linked to the filament formation process in resistive RAM devices [5,6]. Studies [7] have shown boron vacancies to be related to the analogous breakdown process in multilayer hBN.

Here we present the results of our investigation into h-BN and a collection of its intrinsic defects. Using density functional theory (DFT), we analyse boron and nitrogen vacancies and interstitials, boron and nitrogen di-vacancies and Stone-Wells defects. We present the charge transition levels, the ground state spin configuration, and the formation energies of the defects.

We use the CP2K software package [8] to implement DFT. This uses a Gaussian type atomic centred basis set and calculates electronic structure in the gamma point. We use the PBE GGA functional to estimate exchange and correlation energies. The calculations are done in 6x6x4 supercells in periodic boundary conditions. This particular cell expansion was used to give a K-point spacing which would accurately represent the HOMO and LUMO states [9].

We calculate each defect in various charge states. For example, the boron vacancy is found to have 3 charge states: 0, -1, and -2. Neutral boron vacancies introduce unoccupied states in the bottom half of the band gap. Nitrogen vacancies introduce a level 1.6 eV below the CBM. Divacancies are found to have positive binding energy. In particular, the formation of a 'molecular bridge' in interlayer divacancies increases their stability. For example, in the lowest energy configuration of an interlayer boron divacancy, two N atoms form a N-N bridge across the layers. This greatly deforms the surrounding structure and reduces the energy required to form a boron vacancy-interstitial pair. The structure and dynamics of such defects may play a significant role in the breakdown of hBN in nanoelectronic devices.

[1] Dean, Cory R., et al. "Boron nitride substrates for high-quality graphene electronics." *Nature nanotechnology* 5.10 (2010): 722.
[2] Song, Li, et al. "Large scale growth and characterization of atomic hexagonal boron nitride layers." *Nano letters* 10.8 (2010): 3209-3215.
[3] Chen, Ying, et al. "Boron nitride nanotubes: pronounced resistance to oxidation." *Applied physics letters* 84.13 (2004): 2430-2432.
[4] Watanabe, Kenji, Takashi Taniguchi, and Hisao Kanda. "Direct-bandgap properties and evidence for ultraviolet lasing of hexagonal boron nitride single crystal." *Nature materials* 3.6 (2004): 404.
[5] Padovani, A., et al. "A microscopic mechanism of dielectric breakdown in SiO2 films: An insight from multi-scale modeling." *Journal of Applied Physics* 121.15 (2017): 155101.
[6] Bradley, Samuel R., Alexander L. Shluger, and Gennadi Bersuker. "Electron-injection-assisted generation of oxygen vacancies in monoclinic HfO 2." *Physical Review Applied* 4.6 (2015): 064008.
[7] Pan, Chengbin, et al. "Coexistence of Grain-Boundaries-Assisted Bipolar and Threshold Resistive Switching in Multilayer Hexagonal Boron Nitride." *Advanced Functional Materials* 27.10 (2017).
[8] VandeVondele, Joost, et al. "Quickstep: Fast and accurate density functional calculations using a mixed Gaussian and plane waves approach." *Computer Physics Communications* 167.2 (2005): 103-128.
[9] Kharche, Neerav, and Saroj K. Nayak. "Quasiparticle band gap engineering of graphene and graphone on hexagonal boron nitride substrate." *Nano letters* 11.12 (2011): 5274-5278.

Electron-Microscopy and -Spectroscopy of Defects in 2-D Materials

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Recent advances in electron microscopy enable direct visualization of sites of individual atoms in materials as well as disclosure of their chemical nature and electronic structure. The advent of new generation aberration corrected, monochromated (scanning) transmission electron microscopes has made it possible, by combining atomic resolution imaging and spectroscopy as well as DFT modelling, to uncover atomic-scale morphology, constellations of defects, lattice impurities and ad-atoms in materials, as well as their influence on the surrounding electronic bandstructure.

This talk will focus on the revelation of the structure and dynamics of point defects (e.g., foreign-substitutional, interstitial and ad-atoms) and also line defects in 2-D materials (graphene and 2-D transition metal dichalcogenides) [1-3] via high resolution (S)TEM; it will also touch on the assessment of the (opto)electronic properties of defects via electron energy loss spectroscopy carried out in the (S)TEM [4,5], all on the atomic scale. Issues relating to these defects are particularly vital for applications of 2-D materials in opto-electronics, and concern, e.g., the interaction of 2-Ds with metals (for electrical contacting) [6,7] and lattice doping via ion implantation (for Fermi level tailoring) [8,9], as well as collective charge carrier behaviour (plasmons) and tailoring of the latter through the presence of impurity atoms and defects [10]. (S)TEM investigations have furthermore been extended to structural and electronic studies of ferro-electric domain walls, identifying the latter by sub-atomic displacements of the atoms when they form electric dipoles along such boundaries [11], and assessing possibilities to control their formation and mobility with regards to applications in electronic switching. Creation of such boundaries is now being attempted in 2-D materials where they constitute line defects.

[1] R. Zan, U. Bangert, Q. Ramasse and K. S. Novoselov, Nano Letters,12 (2012) 3936.
[2] H.-P. Komsa, S. Kurasch, O. Lehtinen, U. Kaiser and A. V. Krasheninnikov, Phys. Rev. B **88** (2013) 035301
[3] L. Nguyen et al., ACS Nano 2017, 11, (2017) 2894
[4] Q. Ramasse, C. R. Seabourne, R. Zan, D. M. Kepaptsoglou, U. Bangert and A. J. Scott, Nano Lett., **13** (10) (2013) 4989.
[5] D. Kepatsoglou, T. Hardcastle, C. Seabourne, U. Bangert, R. Zan, J. Amani, H. Hofsäss, R. Nicholls, R. Brydson, A. Scott and Q. Ramasse, ACSNano, **9** (11) (2015) 11398.
[6] Q. M. Ramasse, R. Zan, U. Bangert, D. W. Boukhvalov, Y.-W. Son and K. S. Novoselov, ACS Nano 6 (5) (2012) 4063.
[7] R. Zan, U. Bangert, Q. Ramasse, K. S. Novoselov, Nano Letters 11(3) (2011) 1087.
[8] U. Bangert, W. Pierce, D. M. Kepaptsoglou, Q. Ramasse, R. Zan, M. H. Gass, J. A. Van den Berg, C. B. Boothroyd, J. Amani and H. Hofsäss, Nano Letters 13 (10) (2013) 4902.
[9] U. Bangert . A. Stewart, E. O'Connell, E. Courtney, Q. Ramasse, D. Kepaptsoglou, H. Hofsäss, J. Amani, S.-S. Tu and B. Kardynal, Ultramicroscopy, 176 (2017) 31.
[10] U. Bangert, W. Pierce, C. Boothroyd, C.-T. Pan and R. Gwilliam**,** Nature Scientific Reports www.nature.com/articles/srep27090.
[11] C.-L. Jia, S.-B. Mi, K. Urban, I. Vrejoiu M. Alexe and D. Hesse, Nature Materials 7 (2008) 57.

Ion and electron beam modification of graphene

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Heteroatoms in the graphene lattice can drastically alter its electronic, mechanical and chemical properties. These dopants can be introduced either during materials growth, or using a separate modification route. Directly observed substitutions have thus far been limited to incidental Si impurities, and B, N, P dopants. We present here two separate studies: the heaviest reported impurity to date, namely implanted Ge ions, and the electron-beam driven dynamics of P dopants in monolayer graphene.

In the first study, we implanted low-energy $^{74}Ge^+$ ions into single-layer graphene [1]. Although sample contamination introduced during irradiation remains an issue, atomic resolution scanning transmission electron microscopy (STEM) imaging and quantitative image simulations reveal that Ge can either directly substitute single carbon atoms, bonding to three carbon neighbors in a buckled out-of-plane configuration, or occupy an in-plane position in a vacancy.

In the second study, we employed STEM to observe various dynamics of P dopants in graphene, namely direct exchange and Stone-Wales transitions, knock-out of a C neighbor, and replacement of a P atom by C [2]. We also demonstrate the possibility of electron-beam manipulation of P in graphene, although this is more challenging compared to Si.

[1] M. Tripathi, A. Markevich, R. Böttger, S. Facsko, E. Besley, J. Kotakoski and T. Susi, arXiv:1802.04660 (2018)
[2] C. Su, M. Tripathi, Q. B. Yan, Z. Wang, L. Basile, G. Su, M. Dong, J. Kotakoski, J. Kong, J.C. Idrobo, T. Susi and J. Li, arXiv:1803.01369 (2018)

Spectral properties of radiation-induced near-cluster color centers in LiF, NaF and MgF$_2$ nanocrystals

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Dielectric crystals, pure and doped with intrinsic radiation-induced point defects are widely used in various technologies. Recently in nanocrystals (NCs) and near-surface layers of LiF were found radiation CCs, which have early unknown spectral characteristics [1, 2]. It was shown that the presence of nanoclusters is a prerequisite for the formation of near-clusters radiation color centers with specific optical properties [3]. The possibility of creating near-clusters color centers in other crystals is demonstrated in this work. Sodium and magnesium fluorides (NaF and MgF$_2$) crystals were chosen for these experiments.

Samples of NaF and MgF$_2$ in the form of NCs with sizes less then 1 μ m were used. Radiation defects were created by gamma rays from a ^{60}Co source irradiating the samples at liquid nitrogen temperature (T_{irr} = 77 K). Photoluminescence and absorption characteristics are recorded for the samples unfrosted and annealed at room temperature.

Radiation defects with absorption and photoluminescence characteristics, which are significantly different from of previously known those for defects in bulk crystals, have been detected in NaF and MgF$_2$ nanocrystals. It was determined that in these crystals several different types of near-cluster color centers are formed. The luminescence lifetimes of these defects were measured. It is necessary to study changes in non-optical characteristics of materials in which nanoclusters are present.

[1] A.P. Voitovich, V.S. Kalinov, A.P. Stupak, A.N. Novikov, L.P. Runets J. Lumin. 157 (2015) 28
[2] A.P. Voitovich, V.S. Kalinov, M.V. Korzhik, E.F. Martynovich, L.P. Runets, A.P. Stupak Radiat. Eff. Def. Solids 168 (2013)130
[3] A.P. Voitovich, P.A. Loiko, X. Mateos, L.P. Runets, J.M. Serres, A.P. Stupak J. Lumin. 188 (2017) 75

Disorder in multi-band superconductors

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Determination of the symmetry of the superconducting order parameter is the most important and at the same time the most complicated step in elucidating the mechanism of superconductivity. One of the recent approach is the systematic study of the evolution of properties of a superconductor to introduced disorder. In this talk the effect of disorder in multiband superconductors (such as Fe-based pnictides) will be reviewed [1,2]. It will be shown that impact of impurities in multiband superconductors is beyond of a common wisdom: the impurities in s+-superconductors suppress T_c in the same way as paramagnetic ones in common superconductors, and vice versa magnetic impurities act as nonmagnetic ones. Impurities (nonmagnetic as well as magnetic) themselves can give rise new phenomena like change of the symmetry of superconductive order parameter. As a result, intrinsically phase-insensitive experimental methods like tunneling, ARPES, terahertz spectroscopy may be used for revealing of information about the underlying order parameter symmetry. Finally an investigation of a $Ba(Fe_{0.9}Co_{0.1})_2As_2$ thin film by THz spectroscopy and stepwise proton irradiation will be presented [3]. The evolution of the optical conductivity with irradiation dose is explained by the change from sign-reversed (s±) to sign-preserved (s++) symmetry. It signals that s± symmetry is realized in the pristine sample. Summarizing, in the talk it will be shown that systematic study of the response to introduced disorder to a superconductor is a phase-sensitive tool to probe the order parameters of superconductors.

[1] D.V. Efremov, M.M. Korshunov, O.V. Dolgov, A.A. Golubov, P.J. Hirschfeld, Phys. Rev. B 84, 1805512R (2011.
[2] D. V. Efremov, S.-L. Drechsler, H. Rosner, V. Grinenko, and O. V. Dolgov, Phys. Status Solidi B. doi:10.1002/pssb.201600828 (2017)
[3] Micha Benjamin Schilling, Andreas Baumgartner, Boris Gor- shunov, Elena Zhukova, Valery Dravin, Kiril Mitsen, Dmitri Efremov, Oleg Dolgov, Kazumasa Iida, Martin Dressel, Sina Zapf, Phys. Rev. B 93, 174515 (2016)

Vacancy defects with trapped adatoms in epitaxial graphene on Ni(111)

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Dynamically acquired high-resolution scanning tunneling microscopy (STM) images and numerical simulations have recently allowed us to identify individual nickel (Ni) adatoms temporarily attached at the edges of growing graphene flakes on Ni(111) [1]. The analysis of static STM images in the formed epitaxial graphene shows the presence of point-like defects similar for their apparent height and lateral dimensions, which we attribute to vacancies in the carbon (C) network, partially filled with substitutional Ni atoms trapped during the growth [2]. We have modeled in details defects with different shapes, containing up to five C vacancies and three trapped Ni adatoms, and studied their structure and properties using first-principles density functional theory simulations. The energetics and the comparison between experimental and simulated STM images allow to identify most of the observed defects, and to extract some general trend concerning their stability and their abundance. At variance with pristine graphene which is inert, these defects are active centers for interaction with small molecules of environmental importance such as carbon monoxide. [3]

[1] L.L. Patera, F. Bianchini, C. Africh, C. Dri, G. Soldano, M.M. Mariscal, M. Peressi, and G. Comelli, Science **359** (2018) 1243
[2] L.L. Patera, C. Africh, R.S. Weatherup, R. Blume, S. Bhardwaj, C. Castellarin-Cudia, A. Knop-Gericke, R. Schloegl, G. Comelli, S. Hofmann, and C. Cepek, ACSNano **7** (2013) 7901
[3] V. Carnevali et al., in preparation.

TO HAVE (KONDO EFFECT) AND HAVE NOT: RENORMALIZATION AND SCALING

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We discuss the appearance of the Kondo effect in the framework of a general model, describing a quantum impurity with degenerate energy levels, interacting with a gas of itinerant electrons and derive scaling equation to the second order for such a model. If the interaction is presented as

$$V = \sum_{p\pi} G_p \otimes \Gamma_\pi c_{p\pi} \tag{1}$$

where G_p is an operator acting on the state of the impurity, and Γ_π is an operator acting on the internal state of the itinerant electron, the scaling equation can be presented as

$$\frac{dc_{p\pi}}{d\,ln\Lambda} = -\frac{1}{2}\rho \sum_{st\sigma\tau} f_{st}^p \varphi_{\sigma\tau}^\pi c_{s\sigma} c_{t\tau} \tag{2}$$

where f_{st}^p and $\varphi_{\sigma\tau}^\pi$ are the structure constants of the Lie algebras realised by the operators G_p and Γ_π respectively, ρ is the density of states (DOS) for itinerant electrons, and $\Lambda = D/D_0$ is the ratio of the renormalized itinerant electrons band width and the original one.

Being applied to the spin-anisotropic Kondo model

$$\text{V} = J_i S^i \sigma^i \tag{3}$$

where S^i is the spin of the impurity and σ^i is the Pauli matrix, describing spin of the itinerant electron. the scaling equation takes the form

$$\frac{dJ_i}{d\,ln\Lambda} = -2\rho J_j J_k \tag{4}$$

where i, j, k is an arbitrary permutation of Cartesian indexes. Equation (4) is generalized for the case of the power law DOS for itinerant electrons, and solved analytically in terms of elliptic functions.

We also introduce the anisotropic Coqblin--Schrieffer model, apply the general method to derive scaling equation for that model for the power law DOS, and integrate the derived equation analytically.

[1] E. Kogan, K. Noda, and S. Yunoki, Phys. Rev. B 95, 165412 (2017).
[2] E. Kogan, arXiv:1801.0523; Journal of Physics Communications, accepted for publication.

First-principles study of defect complexes in Ti-doped sapphire

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First-principles calculations have been performed [1] to study the formation of defect complexes in Ti doped α-Al$_2$O$_3$ crystals. The formation energies of isolated Ti^{3+} and Ti^{4+} defects, pairs, triples, and quadruples of Ti ions and Al vacancies were computed under different equilibrium conditions of Al-Ti-O related phases. Taking into account the charge neutrality of the whole system, we determine the equilibrium concentrations of simple and complex defects as well as the total equilibrium concentration of Ti in an α-Al$_2$O$_3$ crystal. A universal relation between equilibrium concentrations of isolated and complex defects is obtained. It is shown that the equilibrium concentration of complex defects can be on the same order of or even larger than the concentrations of isolated substitutional Ti^{3+} and Ti^{4+} defects.

The problem of control of the concentration of Ti^{3+}-Ti^{4+} complexes in Ti doped sapphire is addressed. It is believed that such complexes reduce the laser efficiency of Ti:sapphire. It is shown that the ratio of the concentration of Ti^{3+}-Ti^{4+} complexes to the concentration of isolated Ti^{3+} defects is proportional to the concentration of isolated Ti^{4+} defects and depends exponentially on the binding energy of a Ti^{3+}-Ti^{4+} pair. The binding energy is independent of the chemical potentials of atoms in Ti doped α-Al$_2$O$_3$. The concentration of isolated Ti^{4+} depends on the chemical potentials of atoms and, therefore, it is determined by the equilibrium conditions between the phases in the Al-Ti-O ternary system. Under transition from the oxidized to the reduced conditions the concentration of isolated Ti^{4+} defects decreases.

We show that the ratio of the Ti^{3+}-Ti^{4+} to Ti^{3+} defects can be also changed by co-doping of Ti:sapphire with other dopants. Such dopants should form positively or negatively charged defects and their formations energies should be on the same order of or smaller than the formation energy of Ti^{4+} defects. The dopants that form the positively charged defects decrease the concentration of isolated Ti^{4+} ions, while dopants that form negatively charged defects, increase that concentration. To illustrate this effect we consider co-doping of Ti:sapphire with nitrogen, carbon and fluorine impurities. The formation energies of substitutional and interstitial N, C and F ions in different charge states in Ti doped α-Al$_2$O$_3$ are computed under different equilibrium conditions of N-Al-Ti-O, C-Al-Ti-O and F-Al-Ti-O related phases. It is shown that co-doping with nitrogen atoms results in an increase of the concentration of isolated Ti^{4+} and Ti^{3+}-Ti^{4+} defects, while co-doping with fluorine atoms - in a decrease of the concentrations of Ti^{4+} and Ti^{3+}-Ti^{4+}. Carbon atoms form defects with rather high formation energies and co-doping with carbon atoms does not influence significantly the concentration of Ti^{4+} and Ti^{3+}-Ti^{4+}.

Calculations were performed by the pseudopotential method with the use of a strictly localized atom-centered basis set as implemented in the open source SIESTA code based on the density-functional theory approach [2]. The computational facilities of the Joint computational cluster of State Scientific Institution "Institute for Single Crystals" and Institute for Scintillation Materials of National Academy of Sciences of Ukraine incorporated into Ukrainian National Grid were used.

[1] L. Yu. Kravchenko and D. V. Fil, Journal of Applied Physics, 123 (2018) 023104.
[2] J. M. Soler, E. Artacho, J. D. Gale, A. Garcia, J. Junquera, P. Ordejon, and D. Sanchez-Portal, J. Phys.: Condens. Matter 14 (2002) 2745.

Friday

13 July

09:00 - 11:20 Session 12   Chair: U. Bangert

09:00   K. Kaasbjerg (Danish Technical University, Denmark)
A unified theory for quasiparticle interference from defects in two-dimensional materials

09:40   A. Sinner (University Augsburg, Germany)
Transport in systems with nodal degeneracy

10:00   M. Naik (Indian Institute of Science, India)
CoFFEE: Corrections for Formation Energy and Eigenvalues for charged defect simulations

10:20   G. Seifert (TU Dresden, Germany)
Defects in MoS$_2$ monolayers – repair, doping and functionalization

11:00   Closing

11:30   **ICTP Colloquium**
Manipulating many quanta one by one: molecules of light and 51 atomic qubits
Vladan Vuletić, MIT

13:00 - 13:30 Lunch and Departure

A unified theory for quasiparticle interference from defects in two-dimensional materials

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Quasiparticle interference (QPI) measured by low-temperature scanning tunneling spectroscopy (STS) and accompanied by a Fourier transform analysis (FT-STS) provides unique insight into defect-induced scattering mechanisms inside and between the valleys in two-dimensional (2D) materials. Here I present a general T-matrix based framework for the calculation of FT-STS spectra which, in combination with atomistic DFT calculations of the defect scattering potential, allows for detailed modeling of FT-STS spectra for "realistic" defects such as, e.g., atomic vacancies, adatoms and substitutional atoms [1, 2].

In monolayer transition metal dichalcogenides (TDMs; MX_2), atomic vacancies are commonly believed to be a source of pronounced intervalley scattering, thereby presenting a serious obstacle for applications exploiting their unique valley-contrasting properties. However, as I here show, the symmetry of the defect site gives rise to selection rules which protects against intervalley scattering. In the conduction-band FT-STS spectra this manifests itself by a $K \leftrightarrow K'$ intervalley peak which is missing for X vacancies, while appearing clearly for M vacancies. These findings put the recent observations of absent $K \leftrightarrow K'$ intervalley peaks in QPI experiments [3, 4] in a new perspective.

In graphene (and silicene), the chiral nature of the states leaves clear fingerprints in the FT-STS spectra [5, 6]. For example, the central $q=2k_F$ backscattering ring around at the Γ point is strongly suppressed when trigonal warping is small -- this in spite of the fact that atomic defects often break the A,B sublattice symmetry thus allowing for backscattering. The reason for this apparent paradox as well as the reappearance of the backscattering ring at the Bragg points [5,6] emerges straight forwardly from our unified theory. As I furthermore demonstrate, resonant scattering due to defect-induced localized states on the Dirac cone strongly modifies this picture by introducing a hitherto unexplored variant of the backscattering ring at the center of the Brillouin zone.

[1] K. Kaasbjerg *et al.,* Phys. Rev. B 96, 241411(R) (2017).
[2] K. Kaasbjerg *et al.,* in preparation.
[3] H. Liu *et al.*, Nature Commun. 6, 8180 (2015).
[4] M. Yankowitz *et al.*, Phys. Rev. Lett. 115, 136803 (2015).
[5] P. Mallet *et al.*, Phys. Rev. B 86, 045444 (2012).
[6] D. Dombrowski *et al.*, Phys. Rev. Lett. 118, 116401 (2017).

Transport in systems with nodal degeneracy

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We study the DC conductivity of a weakly disordered 2D electron gas with two bands and spectral nodes, employing the field theoretical version of the Kubo-Greenwood conductivity formula. Disorder scattering is treated within the standard perturbation theory by summing up ladder and maximally crossed diagrams. The emergent gapless diffusion modes determine the behavior of the conductivity on large scales. We find a finite conductivity with an intermediate logarithmic finite-size scaling towards smaller conductivities but do not obtain the logarithmic divergence of the weak-localization approach. Our results agree with the experimentally observed logarithmic scaling of the conductivity in graphene with the formation of a plateau near the universal conductivity. We extend our analysis by including effects of anisotropy on hexagonal lattices.

[1] A. Sinner and K. Ziegler
Two-parameter scaling theory of transport near a spectral node
Phys. Rev. B 90, 174207 (2014).

[2] A. Sinner and K. Ziegler
Finite-size scaling in a 2D disordered electron gas with spectral nodes
J. Phys.: Condens. Matter 28, 305701 (2016).

[3] A. Sinner and K. Ziegler
Conductivity of disordered 2d binodal Dirac electron gas: Effect of the internode scattering
Phil. Mag. (2018)

[4] A. Sinner and K. Ziegler
Corrections to the self-consistent Born approximation for Weyl fermions
Phys. Rev. B 96, 165140 (2017).

CoFFEE: Corrections For Formation Energy and Eigenvalues for charged defect simulations

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Charged point defects in materials are widely studied using Density Functional Theory (DFT) packages with periodic boundary conditions. The formation energy and defect level computed from these simulations need to be corrected to remove the contributions from the spurious long-range interaction between the defect and its periodic images. To this effect, the CoFFEE code implements a generalized Poisson solver based on the Freysoldt-Neugebauer-Van de Walle [1] (FNV) correction scheme with a model Gaussian charge distribution. Tools to compute the potential alignment terms in the FNV scheme are also provided with the package. The corrections can be applied to charged defects in a complete range of material shapes and size: bulk, slab (or two-dimensional materials), wires and nanoribbons. The code is written in Python and features MPI parallelization and optimizations using the Cython package for slow steps. Our implementation can be used alongside any DFT package.

Program files: http://www.physics.iisc.ernet.in/~mjain/pages/software.html

[1] C. Freysoldt, J. Neugebauer, and C. G. Van de Walle, Phys. Rev. Lett. 102 (2009) 016402

Defects in MoS_2 monolayers – repair, doping and functionalization

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The control of defects plays a crucial role for the application of MoS_2 monolayers (MLs) in electronic devices. The most important defects are sulfur vacancies. Recent experimental and theoretical studies indicate that thiols (R-SH) can be used to repair sulfur vacancy defects in MoS_2 MLs. Using density functional theory (DFT) we demonstrate how the thiol repair mechanism process can be understood. The interaction with the thiols and possible reaction paths for the repair mechanism are presented. Despite of the repair mechanism the application of thiols as functionalization and doping agents is shown. The electronic structure of the systems is discussed in detail.

ICTP COLLOQUIUM

Friday 13th July 11:30am

Manipulating many quanta one by one: molecules of light and 51 atomic qubits

Vladan Vuletić, MIT

Recent years have seen a remarkable development in our ability to manipulate matter and light at a quantum level. Quantum simulators with individual trapped atoms are becoming a reality, and quantum computing is on the verge of becoming experimentally viable. Of particular interest are tunable strong interactions between atoms that can be used to experimentally implement and control entangled many-body states. Highly excited, metastable atomic Rydberg states can be used to implement controllable long-distance interactions between individual quanta. I will discuss two applications: By coherently coupling light to Rydberg excitations in a dense atomic medium, we have realized a highly nonlinear optical medium where the interactions between individual photons are so strong that two photons can even form a bound state. I will also discuss the use of Rydberg interactions to realize a many-atom quantum simulator with up to 51 individually trapped atoms, where we have observed a quantum phase transition towards a state with antiferromagnetic order, as well as long-lived many-body oscillations after a sudden quench.

Posters

Multiferroic order and magnetoelectricity in mesocrystalline pyrochlore-spinel composite

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Binary phase of naturally favored displacively disordered pyrochlore and structurally identical Fe dominated spinel was studied in the $Bi_2O_3-Nb_2O_5-2MnCO_3-Fe_2O_3$ system [1]. The spinel gains were dispersed throughout the microstructure in mesocrystalline like grains [2]. X-ray diffraction pattern showed presence of normally forbidden 442 reflection which is attributed to appear as a result of displacive disorder of the A_2O' framework of the cubic pyrochlore ($A_2O'.B_2O_6$) where A and B is a larger and smaller cation, respectively [3,4]. The two phases were located by electron probe microanalyzer, high resolution transmission electron microscope as well as by means of Raman spectra. Both polar and magnetic ordering was observed at the room temperature. The system besides hosting the two contrasting orders exhibited a self biased magnetoelectric coefficient of 127mV/cm Oe. The study brings to fore the natural crystallization of pyrochlore and spinel phase [1,2]. Both pyrochlore and spinel lattice posses analogously similar triangular lattice and stabilize in cubic Fd3m space group. The study infuses interest in the composite multiferroics of similarly structured phases of pyrochlore and spinel for realization of a room temperature multiferroic magnetoelectric composite.
[5].

References :

1. R. A. U. Rahman, P. Schmid-Beurmann and R. Murugan, *J. Mater. Chem. C* 4,7766 -7774 (2016).

2. R. A. U. Rahman, P. Schmid-Beurmann and R. Murugan , *J. Alloys Compd.* 763, 409-420 (2018).

3. I. Levin, T. G. Amos, J. C. Nino, T. A. Vanderah, C A. Randall and M. T. Lanagan*, J. Solid State Chem.,* 168, 69-75 (2002).

4. M. A. Subramanian, G. Aravamudan, and G. V. Subba Rao, *Prog. Solid. State Chem.* 15, 55 (1983).

5. C.-W. Nan et al., *J. Appl. Phys.* 103,031101 (2008).

Influence of N-doping on the Optical Absorption of Carbon Nanotubes

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The use of substitutional nitrogen doping of carbon nanotubes to tailor their electronic and catalytic properties has been an area of intensive research for the past decade [1-3]. A full understanding of the influence of nitrogen doping on the electronic and optical properties of SWNTs requires a combined theoretical and experimental approach. In this work, we combine time-dependent density functional theory (TDDFT) calculations with optical absorption spectroscopy and XPS to systematically characterize the influence of N-doping concentration on the optical absorption of SWNTs. Specifically, we consider the influence of Pyridinic and Pyrrolic N-doping on the optical and electronic properties of SWNTs. These results will motivate further studies on the chirality dependent influence of N-doping on the optical and electronic properties of SWNTs.

[1] Scardamaglia, M., Amati, M., Llorente, B., Mudimela, P., Colomer, J., Ghijsen, J., Ewels, C., Snyders, R., Gregoratti, L. and Bittencourt, C. (2014). Nitrogen ion casting on vertically aligned carbon nanotubes: Tip and sidewall chemical modification. Carbon, 77, pp.319-328.

[2] Mowbray, D., Paz, A., Ruiz-Soria, G., Sauer, M., Lacovig, P., Dalmiglio, M., Lizzit, S., Yanagi, K., Goldoni, A., Pichler, T., Ayala, P. and Rubio, A. (2016). Disentangling Vacancy Oxidation on Metallicity-Sorted Carbon Nanotubes. The Journal of Physical Chemistry C, 120(32), pp.18316-18322.

[3] Ruiz-Soria, G., Pérez Paz, A., Sauer, M., Mowbray, D., Lacovig, P., Dalmiglio, M., Lizzit, S., Yanagi, K., Rubio, A., Goldoni, A., Ayala, P. and Pichler, T. (2014). Revealing the Adsorption Mechanisms of Nitroxides on Ultrapure, Metallicity-Sorted Carbon Nanotubes. ACS Nano, 8(2), pp.1375-1383.

Interconnection of charge neutrality level with electronic Structure and p-d hybridization and its modification upon electronic excitations

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Undoped and tin doped cadmium oxide (CdO) based thin films are irradiated by 84 MeV Si^{6+} and 120 MeV Ag^{9+} ions. In the present work the charge nutrality level (CNL) [1] in highly conducting CdO thin films is demonstarted by the observed variation in the band gap upon annealing and doping. The increase in crystallite size with tin doping is a signature of decrease of CdO stoichiometry by substitutional replacement of Cd with Sn. Each Cd^{2+} ions are substituted by Sn^{2+} ions with reduction of Sn^{4+} via creating oxygen vacancies in the lattice which also enhnaces the carrier concentration in the tin doped thin film [2]. The band gap enhancement can not be explained by Burstein-Moss Shift (BMS) only but can be explained by formation of charge neutrality level (CNL). The level of local CNL resides at the branch point of virtual gap states (ViGS) generation of which is the consequence of tin doping in CdO lattice. Further investigations using soft x-ray absorption spectroscopy (SXAS) at Oxygen k and Cadmium $M_{4,5}$ edge and the analysis of the spectral features has revealed an evidence of *p-d* interaction between O 2*p* and Cd 4*d* orbitals. After irradiation, the thin films exhibit an unusual band gap enhancement *via* generation of oxygen vacancies due to huge electronic energy deposition inside the lattice by Ag and Si ions. The observed band gap enhancement has been substantiated by an schematic block diagram [3].

[1] P.D.C. King, T.D. Veal, D.J. Payne, A. Bourlange, R.G. Egdell, C.F. McConville, Surface electron accumulation and the charge neutrality level in In2O3, *Phys. Rev. Lett.* 101 (2008) 116808.

[2] A. Das, S.K. Gautam, D.K. Shukla, F. Singh, Correlations of charge neutrality level with electronic structure and pd hybridization, *Sci. Rep.* 7 (2017) : 40843.

[3] Das, Arkaprava, et al. "Virtual gap states induced modifications in charge neutrality level in cadmium oxide thin films." *Materials Research Express* 4.4 (2017): 045901.

Erbium-Doping Wide Bandgap ZnO Semiconductor for Photonics Applications

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The wide bandgap ZnO (~3.37 eV) has a strategic potential in the field of transparent semiconductors. Erbium has a technological appeal for photonic applications due to its optical emissions in the visible and infrared region, which are associated with optical long-distance communications. Spray Pyrolysis Technique (SPT) allows the preparation of good quality thin films with low financial cost. This study is meant to furnish the effects of Er doping on the structural, morphological and optical properties of ZnO thin films synthesized via SPT. In order to investigate the influence of defects, ZnO:Er thin films were grown in several Er-concentrations (up to 5%) on glass substrates, employing two orders of different magnitude in precursor solution molarity. Optical transmittance/absorbance measurements at room temperature showed an average transparency of 85% in the visible optical range with bandgap values close to the expected. X-rays diffraction measurements confirm the growth of polycrystalline wurtzite ZnO:Er thin films with absence of secondary phases and preferentially along the (002) direction which had an increasing of peak intensity as Er-doping increases independently of sample thickness. As-grown samples showed a linear increase of crystallite size by 3 nm by % of inserted-Er (up 2%). Scanning electron microscopy images showed homogeneous surfaces. The samples were annealed at 300°C during one hour and the crystal qualities deteriorates. However, the traces of Er^{3+} incorporation were confirmed by XPS analysis and photoluminescence measurements at 10K for annealed sample 2%Er, which showed an emission at 1530 nm.

Photoluminescence of Ternary and Quaternary Chalcogenide Nanocrystals: Defects or Strong Electron-Phonon Coupling?

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Chemically synthesized semiconductor nanocrystals (NCs) gain growing interest from the viewpoint of basic physics and numerous applications. They have tunable optical properties promising for light-emitting devices and can provide a viable alternative to silicon solar cells and emerging technologies, because they are compatible with cost-efficient roll-to-roll processing and their surface can be functionalized. Colloidal nanocrystals of ternary ($CuInS_2$, $AgInS_2$, Cu_3SnS_4, *etc.*) and quaternary (Cu_2ZnSnS_4, Zn-Cu-In-Se, *etc.*) chalcogenides are being intensively investigated also for applications in catalysis, sensors, and biomedical markers, taking advantage of their high absorption coefficients, nontoxicity, and appropriate band gaps. Compared to other types of NCs, such as CdSe or PbS, their progress in photovoltaics and other applications is slower, because optimizing the synthesis parameters is more complicated and the defect density is higher. Random positioning of defect states in individual NCs is critical for application, because it can lead to fluctuations of energy levels involved in the charge-transfer in photovoltaic and photocatalytic events, as well as in photoluminescence (PL) band broadening. The efficient elimination of undesirable NC defects demands a deep understanding of their origin and location in the crystal lattice.

The large Stokes shift of the PL of above-mentioned ternary and quaternary chalcogenides was traditionally explained based on the recombination via deep donor (D) and acceptor (A) states [1]. The extremely large (~200 meV) FWHM of this PL was explained by a distribution of D and A energies, as well as of D-A distances from each other and from the NC surface. In recent studies of ultrasmall NCs of a broad range of chalcogenide compounds (including II-VI), typically below 2-3 nm in diameter, which also comprise the class of so-called magic-size NCs like $Cd_{33}Se_{33}$, the D-A model of the broad-band NC emission encountered significant difficulties [2-4]. First, the PL quantum yield in these ultrasmall NCs can reach values well above 50%. This is not typical for defect-related emission. Secondly, for NC sizes as small as several lattice constants and a narrow size distribution (practically zero in the case of magic-size clusters), the range of possible D-A distances is very limited and can hardly account for a large dispersion in PL energy. Similarly, the distribution of the D and A energies is expected to be quite narrow in such NCs. It was therefore suggested recently that strong electron-phonon coupling (EPC) can be the reason for the observed extremely large broadening and Stokes shift of the PL bands in small NCs [1]. Particularly, the model of self-trapped excitons was suggested by us for explaining the PL spectra of several compounds [5].

In this contribution, we summarize our new findings on this topic and discuss it from the viewpoint of the above-mentioned theoretical models. The experimental data were obtained for a series of II-VI (CdS, CdSe) and I-III-VI (Ag-In-S) NCs by a number of spectroscopic techniques including besides PL also Raman and X-ray photoemission spectroscopies providing information on phase purity, crystallinity, and EPC strength, composition, element valence states, and ligand shell structure of the NCs. The results obtained and explanation suggested is proposed for a general discussion about the electronic and optical properties of ternary and quaternary chalcogenide NCs.

[1] Chestnoy, N.; Harris, T. D.; Hull, R.; Brus, L. J. Phys. Chem. 90 (1986) 3393.
[2] O. Stroyuk, A. Raevskaya, F. Spranger, O. Selyshchev, V. Dzhagan, S. Schulze, D.R.T. Zahn, N. Gaponik, A. Eychmüller. J. Phys Chem. C (2018) DOI: 10.1021/acs.jpcc.8b00106
[3] V. M. Dzhagan, M. Ya. Valakh, C. Himcinschi, A. G. Milekhin, D. Solonenko, N. A. Yeryukov, O. E. Raevskaya, O. L. Stroyuk, D. R.T. Zahn. J. Phys. Chem. C 118 (2014) 19492.
[4] A.E. Raevskaya, O.L. Stroyuk, D. Solonenko, V. Dzhagan, S.Ya. Kuchmiy, V.F. Plyusnin, D.R.T. Zahn. J. Nanopart. Res. 16 (2014) 2650.
[5] K. E. Knowles, K. H. Hartstein, T. B. Kilburn, A. Marchioro, H. D. Nelson, P. J. Whitham, D. R. Gamelin. Chem. Rev. 116 (2016) 10820.

Influence of moisture on the operation of a mono-crystalline based silicon photovoltaic cell: A numerical study using SCAPS 1D

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Moisture in the form of humidity has a significant impact on the operation of photovoltaic (PV) cells and panels. Moisture is often diffuse through the encapsulant film (Ethylene Vynil Acetate (EVA), Poly Vinyl Butyral (PVB)) or the breathable back-sheet [1,2]. Moisture is known to accelerate the degradation and reduce the performance of a PV while operating in a wet environment [3]. Due to the high cost and the time needed to performed such studies, SCAPS 1D is widely used to simulate and estimate the operation of PV. In this work, we showed the effect of moisture on the operation and performance of a PV, made from monocrystalline silicon.

Namely, the influence of defects and impurities generated by moisture was investigated. We studied the simultaneous effects of Silanlols Si-OH, Hydrogen ions H^+ , and the metallic ions generated from the corrosion of contacts, encapsulant and transparent conducting oxide (TCO) when there is production of acid (Al^{3+} ; Zn^{2+}), or from dust (Fe^{3+}) [4,5].

The numerical simulation showed that : starting with PV cells without moisture, the Field Factor (FF) and the Power Conversion Efficiency (PCE) drop respectively from 82.80 % to 81.78 % and 18.57 % to 11.46 % , when there is moisture in the cell and PVB used as encapsulant. Further degradation of parameters was observed, when the moisture leads to the production of acetic acid on the EVA, or when there is dust having iron (Fe). FF and PCE were further dropped to 79.20 % and 7.04 % respectively, using the same initial photovoltaic cells. Furthermore, a net decrease in key electrical parameters of the PV was observed throughout the study, with P max , J_{SC} , J_{MP} reducing by more than 50%. This study paves the way for the improvement of performance, and the understanding of degradation process in panels used in wet environments and tropical area.

[1] N. Park, C. Han, D. Kim, Microelectronics Reliability 53 (12) (2013) 1922 – 1926.
[2] M. D. Kempe, A. A. Dameron, M. O. Reese, Progress in Photovoltaics: Research and Applications 22 (11) (2014) 1159–1171.
[3] M. Burgelman, P. Nollet, S. Degrave, Thin Solid Films 361 (2000) 527 – 532.
[4] P. Allongue, C. H. de Villeneuve, S. Morin, R. Boukherroub, D. D. Wayner, 40Electrochimica Acta 45 (28) (2000) 4591 – 4598.
[5] N. B. Ahmed, O. Ronsin, L. Mouton, C. Sicard, C. Yepremian, T. Baumberger, R. Brayner, T. Coradin, J. Mater. Chem. B 5 (2017) 2931–2940.

Influence of hydrogen doping on the optical and electronic properties of ZnO

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We have carried out a comprehensive study on the substitutional (HO) and interstitial (Hi) hydrogen doping in ZnO to obtain a better understanding of experimental observations on these defects. In addition, as an intrinsic defect, hydrogen can easily incorporate during growth or annealing of crystal from the environment. Therefore, optical and electronic calculations were performed using GGA and GGA+U based on density functional theory for high concentrations (in the range of 1020 -1022 cm-3) for H doping. The results show that increment or decrement in cell parameters can be due to the type of considered hydrogen charge. However, concentration doesn't have an effect on the electronic properties in the mentioned range of concentration. The optical and electronic calculations revealed that increment in the band gap and transmission of hydrogen doped atoms is due to the existence of HO doping, nor Hi. In addition, HO doped ZnO improves optical transmission in UV range. Therefore, growth of H-doped samples under O-poor conditions leads to better layers for transparent conducting oxide (TCO) and UV applicable materials. In addition, oxygen vacancy (VO) plus interstitial hydrogen (Hi) complex creates two interbands in the band gap of ZnO, so reduces it to about 1.2 eV [1]. This finding can explain decrement in the band gap of synthesized ZnO, which is about 1.4 eV in experimental observations.

[1] F Bustan Afruz. MJ Tafreshi, <u>MR Mohammadizadeh</u> M. Fazli, Comput. Mater. Sci. 143 (2018) 232.

The Frustration in being Odd:
area law violation in local systems.

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We consider anti-ferromagnetic spin chains with a *weak frustration* -just one bond in a large chain-, such as systems with an odd number of spins with periodic boundary conditions. We show that, in certain cases, a new quantum phase of matter arises in these systems. Such phase is extended, gapless, but not relativistic. The low-energy excitations have a quadratic (Galilean) spectrum.

Locally, the correlation functions on the ground state do not show significant deviations compared to the not-frustrated case, but correlators involving a number of sites (or distances) scaling like the system size display new behaviors.

In particular, the Von Neumann entanglement entropy is found to follow new rules, for which neither area law applies, nor one has a divergence of the entropy with the system size.

Such very long range correlations are novel and of potential technological interest.

We display such new phase in a few prototypical chains using numerical simulations and we study analytically the paradigmatic example of the Ising chain. Through these examples we argue that this phase emerges generally in (weakly) frustrated systems with discrete symmetries.

[1] S.M. Giampaolo, F. Ramos, and F. Franchini, *In Preparation*

Molecular dynamics simulations of He ion channeling in Gold nanoclusters

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Ion channeling is a well-known effect in ion irradiation processes, which is a result of ion moving between the rows of atoms. It drastically affects the ion distribution, ion energy-loss and consequently the damage production in the target. Therefore one could derive the ion-channeling pattern out of the energy-loss behavior of ion-target interaction.

Ion channeling effect is studied for a few pure element crystals and also for some compounds in a systematic way [1]. In this work, we focus on nano-structures which are of major importance, due to their high surface-to-volume ratio. Our results, for different gold cluster sizes, show that ion-channeling occurs not only in the principal low-index, but also in other directions in between. The strengths of different channels are specified, and their correlations with sputtering-yield and damage production is discussed.

[1] Nordlund, K., and G. Hobler. "Dependence of ion channeling on relative atomic number in compounds." Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms (2017).

Ab initio modelling of impurity-dislocation interaction in silicon

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Ab initio modelling of interaction of the edge dislocation with O, N, C, B and H impurity atoms in Si are presented. The supercell is composed of 180 Si atoms with dipole of two edge dislocations and with one impurity atom near each of the dislocation cores. The density functional theory in the general gradient approximation (using the software package ABINIT) has been used for numerical calculation. The interaction curves of the edge dislocations with impurity atoms in the silicon are obtained. The form of the interaction curves corresponds to the well-known Lennard-Jones potential (see figures in [1,2]). The equilibrium positions of impurity atoms in the vicinity of the edge dislocation core, and the binding energy of O, N, C, B and H impurity atoms with edge dislocation are calculated (table 1). One can notice following regularity: with increasing atomic number (number of electrons) of the defect the binding energy of this defect with the dislocation is increased also. It can be noted that values of the binding energies are quite large, which indicates the possibility of the impurity atmosphere formation around the dislocation core that is experimentally observed.

The electronic structure of supercell (composed of 180 Si atoms) with dipole of two edge dislocations with O, N, C, B and H impurities for different impurities positions is presented and analyzed (see figures in [1,2]). When the impurity atoms are in the equilibrium position we can observe a partial separation of the impurity subzone from the bottom of the conduction band and the penetration of the Fermi level into the local pseudogap. Such behavior is quite typical and indicates decreasing of the electronic subsystem energy. It should be noted when the total energy of the supercell goes out on the shelf, the forbidden zone is almost disappearing and the impurity peak is located in the conduction band. This effect can be observed for all impurities under consideration.

The following regularities of the obtained spectra can be established. The obtained spectra corresponds to the spectra of pure Si. The forbidden zone of investigated supercell is significantly reduced. For most of the positions of the investigated impurity atoms in the forbidden zone a sharp peak appears near the Fermi level under the conduction band. Analysis of local spectra allows us to associate this narrow peak in the vicinity of the Fermi level with the electronic states of impurity atoms. The intensity and the fine structure of the impurities peaks depends on the position of the impurity atoms.

With help of the Stoner criterion we analyze the results of calculations from the point of the possible formation of band magnetism. According to this criterion the presence of a semi-filled narrow subpeak in the vicinity of the Fermi level is required. Obtained electronic spectra indicate that (in almost all cases of the impurities positions) an impurity peak appears in the forbidden zone of silicon due to the defective structure of the investigated supercell. This impurity peaks (in almost all cases) are semi-completed.

Table 1. Equilibrium position (relative to the center of the supercell) and binding energy of Si supercell.

Impurity	req., a.u.	Eb per 1 atom, eV	Eb per 1 atom, eV
H	18.8	1.89	
B	19.9	4.12	4.5 [3]
C	19.8	4.08	
N	19.9	5.05	3.24 [4]
O	19.75	5.3	3 [5], 3.6 [3]

[1] T.V. Gorkavenko, I.V. Plyushchay, O.I. Plyushchay, V.A. Makara, *J. Nano- Electron. Phys., 9 (2017) 04025.*
[2] T.V. Gorkavenko, I.V. Plyushchay, O.I. Plyushchay, V.A. Makara, *J. Nano- Electron. Phys., 10 (2018) 03074.*
[3] I. Yonenaga, Materials Science in Semiconductor Processing, 6 (2003) 355.
[4] C.R. Alpass, J.D. Murphy, R.J. Falster, P.R. Wilshaw, J. Appl. Phys., 105 (2009) 013519.
[5] K. Sumino, M. Imai, Phil. Mag. A, 47 (1983) 753.

Atomic Scale Investigations of 1D-2D Heterostructures

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Low-dimensional materials exist with different dimensionalities, for example as two-dimensional (2D) atomically thin layers such as graphene and as quasi-one-dimensional (1D) structures such as nanotubes and nanowires. Although they already have interesting properties individually, when combined into stacked heterostructures, held together by van der Waals forces, they enable creating completely new building blocks for novel devices. Graphene, one-atom-thick layer of carbon atoms, with exceptional electronic and mechanical properties has made a lasting mark in the field of material science. Graphene can be rolled into carbon nanotubes (CNT), which have diameters in the range of nanometers while being several micrometers long. Beyond graphene, which is a zero-band-gap semiconductor, an important class of 2D materials are transition metal dichalcogenides (TMDs) that exhibit semiconducting band gaps. 2D TMDs exhibit a three-atom-thick structure, where a transition metal (such as W) layer is sandwiched between two layers of chalcogen atoms (such as S). Similar to carbon nanotubes, also these materials can be rolled up into tubes.

We use aberration corrected scanning transmission electron microscopy (STEM) to study 1D-2D heterostructures of graphene and nanotubes (carbon and WS2) at the atomic level. In CNT-graphene heterostructures, cleaned in the microscope column with laser irradiation, the randomly deposited nanotubes become self-aligned on a suspended extremely clean graphene monolayer due to minimization of the interface energy. The interfacial interaction leads to deformation of nanotubes and wrapping of the graphene around the CNTs. Due to the much larger diameter of the WS2NTs, such deformations are absent in the WS2NT-graphene heterostructures.

Swift heavy ion tracks in polymers

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Information about the dimensions of latent ion tracks in various polymers, initiated by irradiation with swift heavy ions and measured with different experimental techniques, has been obtained from the publicly available research data. The main observed trend is the increase of the square of the ion track radii with electronic stopping power of the ion. Also, various experimental techniques have resulted in different average track sizes, so a rough estimate of the effect on the experimental technique is given. Available experimental data have been compared with an analytical thermal spike model (ATSM). This model has been used before to interpret experimental ion track data in polymers [1, 2]. The model has also been proven universal and applicable in the widest range of insulating and semiconducting materials.

Here we present the most interesting findings related to the ion tracks in PVDF (polyvinylidene fluoride). Some dispersion of the data has been found with respect to the model predictions, but the obtained data follow general trend given by the model. When only a single experimental technique is considered, dispersion of the data is much lower and can be analysed successfully with the ATSM. Finally, we notice the slow ions often acted as fast, suggesting velocity effect is shifted down to 1 MeV/nucleon.

Keywords: ion track, swift heavy ion, polymer, thermal spike model

[1] G. Szenes, Nucl. Instr. Meth. B 155 (1999) 301-307
[2] G. Szenes et al., Nucl. Instr. Meth. B 166 (2000) 933-937

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Energetic and electronic properties of (0001) plane inversion domain boundary in ZnO/GaN heterostructure

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Wurtzite ZnO semiconductor with a wide band gap of ~3.4 eV at room temperature has attracted a great deal of attention for the light emitting applications. High quality of ZnO film can be achieved based on (0001)-GaN/c-sapphire template with a moderate lattice match of 1.9%. Most recently, we reported the two-dimensional growth of both O-polar and Zn-polar ZnO epilayers on Ga-polar GaN by controlling the O/Zn flux during the ZnO nucleation. We pointed out that the polarity of ZnO epilayer can be changed within only one monolayer by plasma assisted molecular beam epitaxy on Ga polar (0001) GaN substrate. In this work, high angle annular dark field (HAADF) and bright field (ABF) imaging techniques are implemented to clarify the detailed interface structure. It's revealed that the boundary is located at a metallic atom layer with the chemical mixtures most probably to occur within the subsequent N/O elements where the reversed polarity initiates. In order to determine the interface properties, we used ab initio techniques as well as molecular dynamics in order to carry out systematical theoretical simulations on this (0001) plane inversion domain boundary (IDB). The starting point was the eight geometric models (named as: H1-H4, T1-T4 IDB) proposed by Kim and Goo and we considered two kinds of interface atom alignments (type-A: -Zn-O-Ga-N-; type-B: -O-Zn-N-Ga-). The results show that the H4 IDB with type-A interface is the most appropriate configuration among all candidates, in agreement with our experimental observation. Interestingly, the investigations of interface chemical bonding characters and the electronic properties indicate a metallic behavior in all the IDBs configuration with the occurrence of two-dimensional hole gas (2DHG) in H IDBs and two-dimensional electron gas (2DEG) in T IDBs, respectively.

[1] X. L. Guo, J. H. Choi, H. Tabata and T. Kawai, Jpn. J. Appl. Phys. Part 2 40 (2001) L177.
[2] M. B. Ullah, V. Avrutin, S. Q. Li, S. Das, M. Monavarian, M. Toporkov, Ü. Özgür, P. Ruterana, H. Morkoç, Phys. Status Solidi RRL 10 (2016) 682.
[3] J. C. Kim and E. Goo, J. Am. Ceram. Soc. 73 (1990) 4.

First Principale Study of Electronic structure Properties of Pd Doped MoS₂ Monolayer

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Two-dimensional transition metal dichalcogenides (TMDCs) such as MoS2, have attracted huge research becuase of thier intriguing physical, optical and electrical properties [1-5]. The single layer of MoS2 is direct band gap semiconductors [5,6]. In this work, first principale study of Pd doped MoS2 monolayer were studied using generalized gradient approximation presented by Perdew-Burke-Ernzerhof PBE-GGA and based on the density functional theory DFT. Density functional theory is a quantum mechanical modeling method used in physics and chemistry to investigate the electronic structure of many-body systems. The many–body Hamiltonian operator that governs the behavior of a system of interacting electrons and nuclei in atomic units takes the form

$$\hat{H} = -\sum_\alpha \frac{\hbar^2}{2M_\alpha}\nabla_\alpha^2 - \sum_i \frac{\hbar^2}{2m_i}\nabla_i^2 + \frac{e^2}{2}\sum_{\alpha,\beta}\frac{Z_\alpha Z_\beta}{|\vec{r}_\alpha - \vec{r}_\beta|} - \frac{e^2}{2}\sum_{i,j}\frac{1}{|\vec{r}_i - \vec{r}_j|} - e^2\sum_{i,\alpha}\frac{Z_\alpha}{|\vec{R}_\alpha - \vec{r}_i|} \qquad (1)$$

where summations over i and j correspond to electrons, and summations over α and β correspond to nuclei. The kinetic energy terms depend on the spatial differential operator ∇, where the αth nuclei, with atomic number Zα, has a mass of Mα. The three dimensional vector positions of the ith electron and αth nuclei are denoted as ri and Rα, respectively. Due to the terms no. 5, the eq. (1) cannot be solved because separation of variable is not possible here. So, the Solution Simplification or Approximation is required such as Kohn Sham theory, Thomas-Fermi-Dirac theory and So on.

Computational calculations have been done by using the Quantum Espresso software. At first a unit cell of MoS2 consists of 2 S atoms and 1 Mo atom was constructed and optimized. A vacuum slab of length 10 Å was used along c axis as to ward off the spurious interaction with its own periodic image. After this, a (4×4) supercell of MoS2 is made consisting of 16 Mo and 32 S atoms. For the self-consistent field (SCF) and density of states (DOS) calculations, A Γ-centered 8 × 8 × 1 and a 16 × 16 × 1 k-point meshes were used, respectively. The electronic wave functions were represented by plane wave basis with a cutoff energy of 300 eV.

In the absence of Pd dopant, our obtained band gap is 1.8 eV. Our calculations show that the band gap of MoS2 decreases in the presence of Pd about 0.8 eV. The single layer of MoS2 indicates generation of no net spin polarization in the absence of Pd. Our clculations shows an interesting trait of net spin polarization being generated due to non-magnetic Pd doping in a non-magnetic single layer of MoS2. We find that total magnetization is equal to 2 μ_B. Therefore, Pd is a good candidate for decreasing the band gap and improvement the magnetic properties of MoS2 monolayer.

[1] K. S. Novoselov, D. Jiang, F. Schedin, T. J. Booth, V. V. Khotkevich, S. V. Morozov, A. K. Geim, Proc. Natl. Acad. Sci. U.S.A.102 (2005)1045.
[2] B. Radisavljevic, A. Radenovic, J. Brivio, V. Giacometti, A. Kis, Nat. Nanotechnology, 6 (2011) 147.
[3] K. F. Mak, C. Lee, J. Hone, J. Shan, T. F. Heinz, Phys. Rev. Lett. 105(2010) 136805.
[4] A. Splendiani, L. Sun, Y. B. Zhang, T. S. Li, J. Kim, C. Y. Chim, G. Galli, F. Wang, Nano Lett.10 (2010) 1271.
[5] Y. Li, C. Cai, B. Sun and J. Chen, Semicond. Sci. Technol. 32 (2017) 105011
[6] T. Li and G. Galli, J. Phys. Chem. C. 111(2007) 16192.
[7] S. Lebegue and O. Eriksson, Phys. Rev. B 79(2009)115409.

Electron Mobility Investigation in Doped Nanoribbons via Phonon Scattering Mechanisms

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Electron mobility, one of the crucial electron transport parameters, is determined for novel nanoribbon like 2D materials in their doped form with doping of lighter elements such as boron, carbon, nitrogen and fluorine. The fascinating possibility to control electronic properties by varying width and edge of nanoribbons attracts scientific society towards research on graphene nanoribbons (GNR) and boron nitride nanoribbons (BNNR) for development of nanoribbon based nanoelectronic devices. Specifically, we have carried out the calculations for electron mobility for boron and nitrogen doped armchair graphene nanoribbon (aGNR) as well as carbon and fluorine doped armchair boron nitride nanoribbon (aBNNR) via electron – acoustical phonon interactions by deformation potential mechanism (ADP mechanism) and piezoelectric scattering mechanism (PZ) under low field and low temperature regime [1-3]. Pristine graphene, with its zero energy band gap, has limitations for its photovoltaic and nanoelectronic applications and hence the interest builds up towards the doped graphene nanoribbon (GNR) with dopant adatoms (e.g. B, N) as it opens up the possibilities of introducing energy band gap [4, 5] so that it would be possible to fabricate graphene based p-n nanodevices as well as the surface acoustic wave sensors and waveguides at nanoscale [6] wherein boron being trivalent and nitrogen being pentavalent impurity introduces the energy band gap. The variation of electron effective mass has been analyzed with doping concentration of carbon and fluorine individually in boron nitride nanoribbon (BNNR) at large temperature scale under the effect of constantly applied low electric field. For the case of doped aGNR, it has been observed that the electron mobility depends on the doping concentration as well as electron effective mass that affects the overall performance of boron and nitrogen doped graphene nanoribbon based p-n device for its energy and photovoltaic applications. The net electron mobility (ADP + PZ) for boron doped aGNR is observed much higher in comparison with nitrogen doped graphene for a particular temperature. In the case of doped aGNR, it has also been observed that the electron mobility increases with boron doping but reduces with nitrogen concentration. The net acoustical phonon limited electron mobility observed almost invariant with doping concentration of carbon for carburized boron nitride nanoribbon whereas that for the case of fluorinated boron nitride nanoribbon diminishes to considerable extent. The results of this study are important for nanoelectronics and spintronic devices.

[1] U.Bockelmann, G.Bastard,Phys.Rev.B 42 (1990) 8947.
[2] M. Lundstrom, Fundamentals of Carrier Transport, (Cambridge Uni. Press), 2000.pp. 56-89.
[3] A. Pandya, P. Jha, Journal of Elec. Materi., 46 (2017) 2340-2346.
[4] Ci L, Song L, Jin C, Jariwala D, Wu D, Li Y, Srivastava A, Wang Z F, Storr K, Balicas L, Liu F, Ajayan P M Nature Mater. 9, (2010) 430.
[5] P. Rani, V. K. Jindal, RSC Adv., 3, (2013) 802.
[6] Qing Peng, Amir R. Zamiri, Wei Ji and Suvranu De, (2012), https://arxiv.org/abs/1107.1448v2.

The role of molarity precursor solution on the properties of ZnO thin films grown by spray-pyrolysis

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Oxides play fundamental role in the current technological and scientific research of semiconductors due to their versatility and robustness. The optical wide bandgap of zinc oxide (ZnO) allows its application in high power electronics and transparent electrodes providing thin films development a strategic topic. Among many techniques, spray pyrolysis is a large scale production method with advantages as low-cost and versatility when considered as a route to produce thin oxide films. Therefore growth parameters are relevant to their morphology and stoichiometry. One key-parameter is the precursor solution which is pulverized on top of substrate.

Here we show the influence of concentration of zinc acetate dehydrate precursor diluted in distilled water. Thin films of ZnO were grown on top of glass and silicon (001) substrates using solutions with molarity between 0.001 to 1. XRD measurements show polycrystalline films with wurtzite structure. Films grown employing low molarity solutions present larger crystallite sizes and the evidence of (002) preferential growth direction. Low-molarity films are visually transparent as compared to high-molarity films which are presented as white films. The morphology of surface is investigated by scanning electron microscopy. XPS is employed to investigate defects states. Photoluminescence evidence the influence of stoichiometry by the red shift of excitonic emission in UV optical range and the increase of visible optical band emission related to oxygen vacancies. The higher quality for low precursor content solutions is attributed to the large free mean path in the surface due to smaller number of metal atoms providing optimum crystallization.

Intrinsic, extrinsic and intrinsic-extrinsic co-doping in TiO$_2$ thin films

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Oxide-based films and nanostructures have emerged as important materials for a wide range of applications such as photovoltaics, optoelectronics and gas sensing. To develop an appropriate understanding of the properties of these oxides, it is necessary to address the material preparation methods and defect probing issues. This work reports on the synthesis processes of TiO$_2$ based transparent conductive films, their stoichiometry control and defect identifying, in relation with their electrical and optical properties. Nb:TiO$_2$ films were deposited by RF co-sputtering from TiO$_2$ and Nb$_2$O$_5$ targets in Ar plasma. The chemical species present in the plasmas used in deposition process were investigated by optical emission spectroscopy, which was later on correlated with the defects structure of the films. Analysis by XPS shed more light on the nature of the vacancies and on the effect of the latter on the optical and electrical properties of the films. In terms of results, we measured electrical resistivity in the range 10^{-2}-10^{-3} Ω.cm for the intrinsically and extrinsically doped films (films doped with oxygen vacancies and Nb^{+5} respectively) while the lowest resistivity was obtained for intrinsically-extrinsically co-doped TiO$_2$ films (7.4×10^{-4} Ω.cm). The films transparency was also actively determined by the defects in the lattice and highly transparent films (65-85 % in the visible range) were obtained by controlling the density of defects. The approach adopted in this work for the generation of oxygen vacancies could be useful for other oxide-based films, where the oxygen vacancies-dependent properties are crucial, for room temperature ferromagnetism and photocatalytic applications.

New data on core structure of freshly introduced a-screw dislocations in GaN

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GaN and other III-nitrides due to their direct wide bandgap and high temperature stability are promising materials for developing of new light-emitting devices (LEDs) and high-power devices. Economically most suitable way to manufacture such semiconductors is to grow them heteroepitaxially on sapphire. Unfortunately, notable differences both in lattice constants and in thermal expansion coefficients between semiconductor and substrate lead to a very high density of threading dislocations (10^{10} cm^{-2} for edge and 10^8 cm^{-2} for screw dislocations), which reduce significantly LEDs efficiency[1].

Nevertheless, recent investigations [2-4] showed that freshly introduced in basal plane (0001) dislocations in GaN could be effective UV light sources of the intensity that exceeds well free exciton one. In particular, in [2,3] it was found that a-screw dislocations in low-ohmic samples exhibited strong luminescence band at 3.15-3.18 eV whereas their intersection nodes luminesced with the other energy of 3.3eV. On the other hand, in semi-insulating GaN [4] the energy of such luminescence line was about 3.346 eV where the dislocations exhibited perfect core structure. An explanation for these results required transmission electron microscopy (TEM) data on core structure of freshly introduced a-screw dislocations in low-ohmic GaN.

For TEM studies samples of low-ohmic, specially undoped GaN crystalline films grown on sapphire on the (0001) plane were used. First, they were mechanically grinded to the thickness less than 100 μm. Then the grid of indentation pricks with step of ~75 μm under a load of ~500mN were applied on the surface with Nano Indenter G200 (Berkovich tip). Finally, the films were thinned to electron transparency and polished with argon ions with PIPS Gatan.

Preliminary overall study of applied samples was performed with TEM Philips CM200 in two-beam conditions. From prick border propagates the grid of dislocation lines stretched in all {1-210} directions with half-loops at their ends. They were identified using g.b criterion as a-screw ones. In the vicinity of the intersection points the a-screw dislocations became bent creating extended nodes. These nodes and dislocations core structure were studied more closely via scanning mode of Zeiss Libra 200FE, which reduced bending contrasts from material, increased transparent thickness and also improved roughness of dislocation lines with use of high angle annular dark field detector(HAADF). It was discovered that dislocations dissociated in two partials of 30°-Shockley type bounding I2 stacking fault ribbons. Two types of the extended nodes were observed: single-triangle and double-triangle ones. The dissociation width of a-srew dislocations was in the ranges 5-7 nm while the radius of the nodes was of about 11-13 nm.

The obtained results allowed to explain the difference in the spectral position of dislocation-related luminescence(DRL) in low-ohmic [2,3], and semi-insulating GaN [4] to be due to different core structure of the dislocation in these two types of the material. The DRL red shift of 0.15 eV in semi-insulating samples was explained with the help of recently developed theory that predicted the existence of attractive conduction band bending at screw dislocations which is absent in deformation potential theory. The theory of the energetics of dissociated screw dislocations is absent up to now and is needed to be developed to explain quantitatively there luminescent properties.

1. Fong Kwong Yam, Li Li Low, Sue Ann Oh, and Zainuriah Hassan, Gallium Nitride: An Overview of Structural Defects, InTech, 2011
2. O. S. Medvedev, O. F. Vyvenko, A. S. Bondarenko, Semiconductors 2015, 49, 1181
3.O.S. Medvedev, O.F. Vyvenko, Phys. Status Solidi RRL, 2017, 1700297
4. M. Albrecht, L. Lymperakis, and O. Neugebauer, Phys. Rev., 2014, B 90, 241201

Growth of V_2O_5 nano-rod thin films for the purpose of conducting layer in various devices

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Transition metal oxides (TMO) are compounds comprising oxygen atoms bound to transition elements. These oxides exhibit phenomenal range of electrical and optical properties, which make them useful in numerous applications such as sensors, solar cells, laser hosts, anti-cancer agents, etc. [1-3]. Moreover, the development of nano-sized structures of TMO's has further widened their applications in each field. The work outlined here focuses on the growth of vanadium pentoxide (V_2O_5) nano-rods on thin glass substrates via two different processes: conventional annealing and microwave sintering. To the best of our knowledge, the microwave sintering has not been applied for the development of V_2O_5 nano-rods. The thin films grown have been characterized for optical and morphological properties. Furthermore, its application in organic solar cells has been investigated.

V_2O_5 thin films of various thicknesses (5 nm-260 nm) were grown on cleaned glass and ITO substrates using thermal evaporation technique keeping the deposition rate between 2-4 Å/s. The deposited films were annealed in a furnace at different temperatures (200-600 °C) and for different time durations (2 hrs – 4 hrs). For microwave sintering, the samples were annealed at different temperatures and durations. The prepared thin films were studied for optical properties using UV-visible spectroscopy, and for morphology study, x-ray diffraction, atomic force microscopy and scanning electron microscopy were employed. Solar cells of the following configuration were prepared ITO/V_2O_5/P3HT:PCBM/Al were fabricated to study the effect of V_2O_5 thickness on the performance of solar cells.

The absorption of V_2O_5 films increased with increase in thickness and also increased with annealing of the samples. The energy band- gap ranged from 1.54-2.45 eV. The as-grown films were amorphous in nature, while annealed films showed crystalline structure. Uniform nano-rods were obtained at temperatures above 400 °C, as shown in the figure. The band-gap of V_2O_5 was found to be suitable for solar cell application and open circuit voltage as high as 0.8 V was achieved, which is higher than PEDOT:PSS based solar cells (0.56 V).

[1] S. Beke, Thin Solid Films, 519 (6) (2011) 1761-1771.
[2] J. Sun, C. Li, Y. Qi, S. Guo and X. Liang, Sensors 16 (2016) 584.
[3] G. Li, C.-W. Chu, V. Shrotriya, J. Huang, and Y. Yang, Applied Physics Letters 88 (2006) 253503.

Ion irradiation-induced easy-cone anisotropy in double-MgO free layers for perpendicular magnetic tunnel junctions

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Interface-induced magnetic phenomena have sustained the latest developments of spin electronics [1,2]. One such phenomenon, the perpendicular magnetic anisotropy (PMA) at the FeCo/MgO interface, is the basis of the perpendicular magnetic tunnel junction (pMTJ) used in spin-transfer-torque magnetic random-access memories (STT-MRAM) [2]. Improved STT-MRAM switching efficiency is expected by setting an easy-cone anisotropy in the pMTJ free-layer [3]. Such an easy cone requires a second-order PMA term, $K_2 < 0$, alongside a first-order $K_1 > 0$, and has been observed in MgO/FeCoB/Ta stacks within a narrow range of FeCoB thicknesses in the crossover from out-of-plane to in-plane anisotropy [4,5,6]. While K_1 stems from Fe-O orbital hybridization [2], the origin of K_2 is likely related to structural and magnetic inhomogeneities such as periodic fluctuations of K_1 [4,5,6]. All those structural properties, and thus the PMA, may be modified by ion irradiation [7].

Here, we demonstrate the control of the anisotropy direction in MgO/FeCoB/X/FeCoB/MgO (X = W or Ta) free-layers by 400 keV Ar^+ irradiation. Ferromagnetic resonance revealed a linear decrease of K_1 with increasing Ar^+ fluence up to 10^{15} cm^{-2}, caused by elemental mixing at the FeCoB/MgO interfaces, which allowed us to induce easy-cone states in 2.6 nm-thick FeCoB free layers, initially with an out-of-plane anisotropy, without increasing the damping.

[1]   F. Hellman et al., Rev. Mod. Phys. 89, no. 2,025006 (2017).
[2]   B. Dieny and M. Chshiev, Rev. Mod. Phys. 89, no. 2, 025008 (2017).
[3]   N. Strelkov et al., Phys. Rev. B 95, 184409 (2017).
[4]   B. Dieny and A. Vedyayev, Europhys. Lett 25, 723 (1994).
[5]   J. Z. Sun, Phys. Rev. B 91, 174429 (2015).
[6]   A.A. Timopheev et al., Phys. Rev. B. 96, 014412 (2017).
[7]   J. Fassbender et al., J. Phys. D: Appl. Phys. 37, R179 (2004).

Investigation of deformation processes in Lithium Fluoride (LiF) and Silicon (Si) crystals caused by external mechanical loading using time-resolved X-ray diffraction method based on adaptive X-ray optics

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The report describes the investigation of irreversible deformation processes in crystalline materials under external loading with appliance of a new X-Ray time-resolved diffraction method based on adaptive X-ray optics. This method allows receiving information about changes in atomic structure recording rocking curves (the dependence of the X-ray radiation intensity on the angle near Bragg angle) by fast tunable X-Ray optic element. This element consists of a piezoelectric monolithic bimorph lithium niobate ($LiNbO_3$) single crystal and a silicon plate with high X-ray optic quality attached to its face. X-ray beam falls on this silicon plate, and when electrical signal is applied to the lithium niobate, the optic element bends, and it becomes possible to control the spatial position of the diffracted X-ray beam [1]. Time resolution of proposed method scales up to microseconds and depending on the brilliance of X-ray source. For now, such adaptive X-ray optic elements for nonmechanical beam control have been successfully tested on laboratory X-ray sources of low power and at synchrotron source in Kurchatov Institute.

Using this technique, the evolution of defect structure of Lithium fluoride (LiF) and Silicon (Si) single crystals in case of vibration in kHz range was observed. The essence of such evolution is defect multiplication, displacement and shifting of atomic planes under influence of kHz vibration, which can be determined by changes in rocking curves parameters. Vibration with kHz frequency in investigated sample is caused by glued piezoelectric transducer of quartz crystal, controlled by external electric field.

The presented approach makes it possible to obtain information about irreversible changes in the crystal structure with a lower time delay compared to existing methods. This technique can be used for operative diagnostics of defects within crystal structure in research and production organizations related to the fabrication of microelectronic components and systems based on crystalline materials.

[1] A.E. Blagov, Y.V. Pisarevskii, A.V. Targonskii, I.A. Eliovich, M.V. Kovalchuk, A.S. Bykov, I.V. Kubasov, M.D. Malinkovich, Instruments and Experimental Techniques. 2016. T. 59. № 5. C. 728-732.

Cobalt impurity in thin dioxide and its influence in hydrogen sensors

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The structure and defects of cobalt doped tin dioxide were investigated using the density functional theory [1]–[4]. The computations were carried out for different concentrations of cobalt (3.125, 6.25, 12.5, and 18.75 at%). It is shown that at the cobalt doping less than 4 at%, the oxygen vacancy occurs at the place of the oxygen bounded by cobalt. It is energetically favorable for oxygen vacancy to occur at the nearest place to cobalt atom. The vacancy forms on the same octahedral. The electron density of states is computed when cobalt creates the states near a conduction band. By further increase in the cobalt concentration, the order of the structure begins to destroy. The structure order of tin dioxide cell is decreased in the case of 12.5 and 18.75% (in atomic percents) cobalt doping.

In the different environment conditions, surface structure changes. The number of oxygen vacancies is increased. This means that reactivity of the surface is changes, and different gases can by adsorped or detected. The adsorption of hydrogen milecule was investigeted by Density Functional Theory. It was found, that the surface is more sensitive to hydrogen molecule, in the case of 3.125 % cobalt doping, than in the undoped case. This result is in common with the experimantal researches [5]□.

[1]   W. Kohn and L. J. Sham, "Self-Consistent Equations Including Exchange and Correlation Effects," *Phys. Rev.*, vol. 140, no. 4A, pp. A1133–A1138, Nov. 1965.

[2]   P. Hohenberg and W. Kohn, "Inhomogeneous electron gas," *Phys. Rev.*, vol. 136, no. 3B, pp. B864–B871, Nov. 1964.

[3]   P. Giannozzi *et al.*, "Advanced capabilities for materials modelling with Quantum ESPRESSO," *J. Phys. Condens. Matter*, vol. 29, no. 46, p. 465901, Nov. 2017.

[4]   P. Giannozzi *et al.*, "QUANTUM ESPRESSO: A modular and open-source software project for quantum simulations of materials," *J. Phys. Condens. Matter*, vol. 21, no. 39, 2009.

[5]   G. Korotcenkov, I. Boris, V. Brinzari, S. H. Han, and B. K. Cho, "The role of doping effect on the response of SnO2-based thin film gas sensors: Analysis based on the results obtained for Co-doped SnO2 films deposited by spray pyrolysis," *Sensors Actuators B Chem.*, vol. 182, pp. 112–124, Jun. 2013.

The simultaneous effects of nanostructures morphology and external electric field on the energy spectrum of donors inside core/shell nanodots

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Deploying a variational calculation, within the effective-mass approach, the impact of an external electric field directed along to the **Oz**-axis on the binding energy of a single donor impurity was examined. The discontinuity of the permittivity, ε_r, and of the particle effective mass, $m_i^*(r)$, at the nano-system boundaries was considered. Deploying the image charge approach, the impact of the surrounding medium on the shallow donor energy spectrum was also taken into account. Our theoretical investigation shows that, for zero electric field and when the shell thickness is taken constant, the increase of the core material size leads to decrease the single donor correlation energy. Further, for a fixed core material size the energy decreases quickly when the shell thickness moves from 0 to 1 nm, while it decreases very slowly when the shell thickness is ranged between 1 nm to 4 nm. On the other hand, we have established that when we turn on an external electric field, the probability density of confined particles tends to move toward the nano-dot border, which naturally redshift the energy spectrum of our nano-system. It was also obtained that the donor stark shift depends not only on the nano-dot size, but also on the surrounding medium.

[1] M. Cristea, E.C. Niculescu, Eur. Phys. J. B 85 (2012) 191
[2] A. Chafai, I. Essaoudi, A. Ainane, F. Dujardin, R. Ahuja, Phys. E 94 (2017) 96.
[3] A. Chafai, F. Dujardin, I. Essaoudi, A. Ainane, R. Ahuja, Superlattices Microstruct. 111 (2017) 976.
[4] L. Shi, Z.W. Yan, Phys. E 98 (2018) 111

Defects of Graphene Oxide Produced by Laser Ablation Method in Different Liquid Environments

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In this work, the effect of liquid environments on the characteristics of carbon nanostructures – in particular, Graphene oxide (GO) – prepared by pulsed laser ablation were studied experimentally. Graphite target was ablated with the second harmonic pulse of Nd:YAG laser, operated at 7 ns pulse width, 5 Hz repetition rate and 532 nm wavelength. 5000 laser pulses were used to produce carbon nanostructures in Liquid nitrogen, deionized water, and cetyltrimethylammonium bromide (CTAB) 0.01 molar. The fluence of laser pulse was 0.7 J/cm^2 with 6 mm diameter. Produced nanostructures were characterized by Raman scattering spectrum, FE-SEM and TEM images, Photoluminescence, and UV-Vis-NIR spectrum. TEM and FE-SEM images show sheet-like morphology with few square micrometer area graphene in all samples. In Raman spectra, the shifts in the G band peaks of samples are due to the oxygenation of produced graphene from graphite target [1]. Furthermore, there are two other peaks in the plot of sample 1, which are attributed to the intrinsic defects of amorphous carbon [2] and formation of nano-diamonds [3]. The exitonic absorption peaks in UV-Vis-NIR spectra are occurred in 300 nm in all samples. Due to the small size of prepared GO nanosheets, most atoms are localized at the surface of samples. These surface atoms can represent some localizing defect sites, owing to unsaturated dangling bonds which behave as carrier trapping sites [4]. The presence of defects in produced GO can provide trapping sites for carriers and leads to quenching of the radiative exitonic recombination. This possibility of recombination through trap sites might be a reason for broadening of trap emission over a wide range of wavelengths which are occurred in PL spectra. Results show that, in our experimental conditions, despite of multilayer graphene oxide nanosheets, deionized water is a capable carrier medium to produce GO sheets. This sample (sample 2) contains the largest sp^2 domain size, the least defects and the lowest possibility of aggregation. Results show that laser ablation method is a capable way to produce graphene based materials [5-7].

[1] S. Stankovich, D. A. Dikin, R. D. Piner, K. A. Kohlhaas, A. Kleinhammes, Y. Jia, Y. Wu, S. T. Nguyen, R. S. Ruoff, Synthesis of graphene based nanosheets via chemical reduction of exfoliated graphite, Carbon 45 (2007) 1558-1565.

[2] S.Y. Lee, M. Yamada, M. Miyake, Synthesis of carbon nanotubes and carbon nanofilaments over palladium supported catalysts, Sci. Tech. Adv. Mater. 6 (2005) 420-426.

[3] S.Z. Mortazavi, P. Parvin, A. Reyhani, Fabrication of graphene based on Q-switched Nd:YAG laser ablation of graphite target in liquid nitrogen, Laser Phys. Lett. 9 (2012) 547-552.

[4] E. Soheyli, R. Sahraei, G. Nabiyouni, pH-dependent optical properties of N-acetyl-L-cysteine-capped ZnSe(S) nanocrystals with intense/stable emissions, Nanopart Res 19 (2017) 92.

[5] N. Tabatabaie, D. Dorranian, Effect of fluence on carbon nanostructures produced by laser ablation in liquid nitrogen, Appl. Phys. A 122 (2016) 558-567.

[6] H. Sadeghi, D. Dorranian, Influence of size and morphology on the optical properties of carbon nanostructures, J. Theor. Appl. Phys. 10 (2016) 7-13.

[7] A. Zamiranvari, E. Solati, D. Dorranian, Effect of CTAB concentration on the properties of graphene nanosheet produced by laser ablation, Opt. Laser Technol. 97 (2017) 209-218.

Intrinsic Point Defects in Bulk ZrS2: A Defect-Tolerant Semiconductor

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Bulk ZrS2 has attracted wide attention due to its unusual electrical, optical, and mechanical properties, which are strongly affected by defects. Using hybrid density functional theory (DFT), we have explored the thermodynamic and optical analysis of intrinsic structural defects in bulk ZrS2. Most of them are donors defects with low formation energies (E_f), indicating their high concentration. However, only Zr vacancy (V_{Zr}) is a shallow acceptor defect with high E_f. Sulfur interstitial (I_S) and sulfur antisite (S_{Zr}) are electrically inactive defects. Donor defects form spontaneously in the p-type sample and their low E_f, push the Fermi level close to the conduction band, indicates that it is impossible to achieve p-type doping with a high concentration of hole carriers. Among all the intrinsic defect, Zr interstitial (I_{Zr}) shows n-type conductivity with very low formation energy, pinning the Fermi level close to the conduction band and thus making ZrS2 as an n-type semiconductor.

A combined first-principles and empirical potential study of first-order Raman scattering in defective MoS$_2$

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Two-dimensional (2D) materials offer interesting and unique properties for devices. The existence of structural defects can play either detrimental or beneficial roles, depending on the targeted application. Raman spectroscopy is known as an important and versatile tool for the characterization and the control of defects. A wide range of scales are covered through first-principles calculations and empirical potential approach, to determine Raman activity at low concentrations, and to specify the role of higher defect concentration and defect disorder respectively. In order to extract relevant modes out of performed calculations, and to yield approximative peak shape, the band unfolding scheme is used. As a result, we find out i) How the peaks from pristine system evolve upon increasing defect concentration? ii) Are the changes common for all point defects or they depend on the defect? iii) How the defect size affects the results, i.e., the vacancy density vs. defect density in the case where one defect con- tains more than one vacancies.

[1] S. Mignuzzi, A. J. Pollard, N. Bonini, B. Brennan, I. S. Gilmore,
    M. A. Pimenta, D. Richards, and D. Roy, Phys. Rev. B 91, 195411 (2015).
[2] F. Zheng and P. Zhang, Computer Physics Communications 210, 139 (2017).
[3] H.-P. Komsa and A. V. Krasheninnikov, Phys. Rev. B 91,125304 (2015).

The spin orbital dynamics properties of vacancy diamond films using enhanced Raman scattering spectroscopy

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We investigated the Raman scattering spectrums of difference residual stress and thickness of diamond/Si films. The spin-orbital dynamics is caused by disordered lattice coupling and electron-phonons in diamond/Si. The diamond films were prepared on a Si substrate by MPCVD with methyl-hydrogen gas mixture. The Raman scattering spectrum of diamond/Si(100) hetero-junction was found as a function of crystal size, orientation, and film thickness. A sharp peak at 1360cm^{-1} is of D graphite sp^2, while the broad peak 1550 cm^{-1} of a broad band mode G, which corresponds to disordered sp^2 hybridization. The transfer of diamond sp^2 content extracted from C=C peak and converted to the sp^3 spin related effect. The diamond/Si(100) density state shows spin-related couple of sp^3, p and d orbital hybridization

[1]   A T.N. Makgato, E. Sideras-Haddad M.A. Ramos,M. García-Hernández, A. Climent-Font, A. Zucchiatti , A. Muñoz-Martin, S. Shrivastava, R. Erasmus, Journal of Magnetism and Magnetic Materials, 413 (2016) 76–80
[2]   J. Michael Boteler, Y. M. Gupta, Phys. Rev.B, 66, (2002)014107
[3]   A.I. Shames,,V.Yu. Osipov, A.E. Aleksenskiy, E. Ōsawa, Diamond & Related Materials 20 (2011) 318–32
[4]   K. Honda,T. Noda, M. Yoshimura,K. Nakagawa, A. Fujishima, J. Phys. Chem. B 108(2004) 16117-16127
[5]   Ala'Eddin A. Saif, P. Poopalan,Optoelectronics and Advanced Materials-Rapid Communivations,**4(12)** (2010)2008-2010
[6]   S. Jin, T. H. Tiefel, M. McCormack, R. A. Fastnacht, R. Ramesh, and L.H. Chen, Science **264** (1994)413
[7]   Y.C. Wang, R Ren, C.L. Chen, Canadian J. of Phys. **83** (2005) 699
[8]   K.Hammerer, M.Wallquist, C.Genes, Phys. Rev. Lett.103,6, (2009)063005.
[9]   G. Balasubramanian, P. Neumann, D. Twitchen, M. Markham, R. Kolesov, N. Mizuochi, J.Isoya, J. Achard, J. Beck, J. Tissler, Nature Materials,8(5), (2009)383-38
[10]   P.Rabl, , Phys. Rev. Lett. 107(6), (2011)063601
[11]   P. W. May, C. A. Rego, C. G. Trevor, E. C. Williamson, M. N. R. Ashfold, K. N. Rosser,N. M. Everitt,Diamond and Related Materials, 3 (1994) 1375- 1380
[12]   Takatoshi Yamada, Atsuhito Sawabe, Satoshi Koizumi , Takaaki Kamio , Ken Okano, Diamond and Related Materials 11 (2002) 257–261
[13]   H. Tanaka, J. Zhang, and T. Kawai, Phys. Rev. Lett. **88** (2002) 027204
[14]   A. Sawa, T. Fujii, M. Kawasaki, and Y. Tokura, Appl. Phys. Lett. **85**, (2004)4073
[15]   C.J. Tang,M.A. Neto, M.J. Soares,A.J.S. Fernandes,A.J. Neves, J. Grácio, Thin Solid Films 515 (2007) 3539–3546
[16]   Sun J R, Appl.Phys. Lett.**101**(15) (2012)152901
[17]   Claire A.McLellan, Bryan A.Myers, Stephan Kraemer, Nano Lett.16,4, (2016),2450
[18]   T. Shardaa,T. Soga , T. Jimbo , M. Umeno Diamond and Related Materials,9,(2000) 1331-1335
[19]   Kim Hee-Dong, Yun Min Ju, Kim Sungho, Journal of the Korean Physical Society,69,3,(2016)439-442
[20]   Choi In Hwan, Park Hyeon Jeong, Journal of the Korean Physical Society,64,9,(2014)1351-1355

Defects in two-dimensional MoTe₂: from point to extended defects

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Defects commonly alter the properties of layered materials e.g. from electronic transport to catalytic activity [1-3]. They also provide an efficient way of engineering, likewise doping in semiconductors [4]. As a result, the detailed atomic structure of defects and their stabilities is of fundamental importance.

Using first-principles calculations combined with high-resolution transmission electron microscopy experiments, we study creation, agglomeration, and evolution of vacancies in monolayer MoTe₂ under electron irradiation. Various types of point and extended defects are studied and their atomic structures and formation energies are determined. The stability of the flower defects and the trefoil-like defects are compared with the line vacancies. Single Te vacancies are found to have a tendency for agglomeration into the vacancy lines. The stability of line defects is also found to be dependent on their orientation and they are energetically more favorable along the zigzag direction. We have also studied the effect of uniaxial and biaxial strain on the stability and dynamics of line defects. The results show that the defects can change the electronic structure which offers new opportunities for defects engineering in this layered materials.

References
[1] M. Ghorbani-Asl, A. N. Enyashin, A. Kuc, G. Seifert and T. Heine, Phys. Rev. B 88 (2013) 245440.
[2] L. Ma, Y. Tan, M. Ghorbani-Asl, R. Böttger, S. Kretschmer, S. Zhou, Z. Huang, A. V. Krasheninnikov, F. Chen, Nanoscale 9 (2017) 11027.
[3] B. Mohanty, M. Ghorbani-Asl, S. Kretschmer, A. Ghosh, P. Guha, S. Panda, B. Jena, A. V. Krasheninnikov, B. Jena, ACS Catal. 8 (2018) 1683.
[4] M. Ghorbani-Asl, S. Kretschmer, D. Spearot, A. V. Krasheninnikov, 2D Mater. 4 (2017) 025078.

A combined experimental and theoretical study of the crystallographic degradation in nearly lattice-matched InAlN layers to GaN

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High Electronic mobility transistors (HEMTs) based on GaN are very important devices for amplification and detection of the microwave power signals. The binary compounds of group III nitride (InN, AlN and GaN) and their alloys are used for numerous applications such as light emitting diode (LEDs), diode laser (LDs) and transistors with high electronic mobility (HEMTs). In particular, the ternary compound InAlN has recently attracted much research interest due to the possibility of lattice matching it to GaN for an indium composition of around 18%. In addition, the higher 2DEG charge density in InAlN/GaN HEMTs results in higher output current density and, potentially, higher power density [i,ii]. Moreover, the band gap of $In_xAl_{1-x}N$ alloys covers the widest range of semiconductor alloy system from 0.67 eV (InN) to 6.2 eV (AlN). Recently, it has been pointed out that, the $In_{0.18}Al_{0.82}N$ alloy is in the immiscibility gap; however, it was claimed also that biaxial strain can modify the miscibility gap [iii]. Therefore, it is important to study the various factors that can influence the indium segregation in these heterostructures.

In this work, we have used a combination of microscopy techniques and theoretical modelling in a detailed study of InAlN layers grown on GaN. The theoretical modelling is carried out using ab-initio methods (DFT), along with molecular dynamics for large systems. The microstructure of the defects was studied by conventional transmission electron microscopy and Scanning transmission electron microscopy at atomic resolution using a JEOL ARM200 microscope for chemical sensitive imaging and local composition. From this investigation, it comes out that the spontaneous degradation of nearly lattice-matched InAlN layers to GaN is based on the effect of native defects that play a critical role on the In segregation and subsequent accumulation of the local strain.

[i] F. Medjdoub et al.,"Can InAlN/GaN be an alternative to high power high temperature AlGaN/GaN devices?" 2006 Int. Electron Devices Meeting (IEDM), 2006, Tech. Digest, 927

[ii] J. W. Chung, O. I. Saadat, J. M. Tirado, X. Gao, S. Guo, and T. Palacios, "Gate-Recessed InAlN/GaN HEMTs on SiC Substrate With Al2O3 Passivation" IEEE Electron Device Lett., vol. 30, no. 9, pp. 904-906, Sep. 2009.

[iii] R. Mohamad, A. Béré, J.Chen, and P. Ruterana, Phys. Status Solidi A 1600752 (2017).

Theoretical study of physical properties of graphene-like ZnO nanosheet in the presence of vacancy deffect

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The isolation of a single layer of graphite, known today as graphene, not only demonstrated amazing new properties but also paved the way for a new class of materials often referred to as two-dimensional (2D) materials. Recently, the interest in ZnO nanostructures has significantly increased owing to their specific structures and properties differ from bulk counterparts, leading to many potential applications [1-3]. Several ZnO nanostructures have been synthesized and characterized, in particular in the form of ultrathin nanosheets [2, 3]. The two-dimensional layered phase of ZnO was firstly predicted by Freeman that ZnO film prefers a graphitic-like structure when the number of ZnO (0001) layers is reduced due to the depolarization of the surface [3].

In this work, we have studied electrical and mechanical properties of graphene-like ZnO monolayer with vacancy defect by using density functional theory (DFT) [4]. Here, DFT is implemented by Quantum Espresso software package [5] based on generalized gradient approximation presented by Perdew-Burke-Ernzerhof (PBE-GGA) [6]. we have shown that vacancy of oxygen results in decreasing the band gap of the system. Moreover, the band gap completely disappears due to the vacancy of oxygen and Zinc atoms in the super lattice. Therefore, we concluded that both types of vacancies result in the metallic behavior of the ZnO nanosheet. Furthermore, our calculation shows that none of vacancy types of Oxygen (V_O) or Zn and O atoms ($V_{Zn,O}$) leads to magnetic state of the system. However, we predict that the Zn vacancy would result in magnetization in the system. Besides, our studies on mechanical properties of the system in the presence of vacancy defects show that stability and mechanical strength are lower than the case of ZnO sheet without any defect.

[1] G. Weirum, et al, J. Phys. Chem. C 114, (2010) 15432.
[2] C. Tusche, H.L. Meyerheim, Kirschner, J. Phys. Rev. Lett. 99 (2007), 026102..
[3] M. Topsakal, Cahangirov, S.; Bekaroglu, E.; Ciraci, S. First-principles study of zinc oxide honeycomb structures. Phys. Rev. B 2009, 80, 235119.
[4] M. John Wills, (2010), Springer series solid state science 167.
[5] P. Giannozzi, *et al*, J.Phys.:Condens.Matter 29, (2017) 465901.
[6] J. Perdew, Y. Wang, Physical Review B 33 (1986) 8800.

Mon 9.07		Tue 10.07		Wed 11.07		Thu 12.07		Fri 13.07	
9:00-9:30	A .Krasheninnikov	*chair:*	*V. Meunier*	*chair:*	*J. Kotakoski*	*chair:*	*G. -D. Lee*	*chair:*	*U. Bangert*
9:30-10:00	T. Michely	9:00-9:40	A. Zobelli	9:00-9:40	M. Nastasi	9:00-9:40	M. Schleberger	9:00-9:40	K. Kaasbjerg
10:00-10:30	T. Susi	9:40-10:20	H.-P. Komsa	9:40-10:20	A. Vantomme	9:40-10:20	D. Golberg	9:40-10:00	A. Sinner
10:30-11:00	H.-P. Komsa	10:20-10:40	M. Scardamaglia	10:20-10:40	Anđelković	10:20-10:40	C. Hofer	10:00-10:20	M. Naik
								10:20-11:00	G. Seifert
11:00-11:30	Coffee break	10:40-11:20	Coffee break	10:40-11:20	Coffee break	10:40-11:20	Coffee break	11:00	Closing
11:30-12:00	M. Nastasi	*chair:*	*P. Bøggild*	*chair:*	*H.-P. Komsa*	*chair:*	*M. Schleberger*	11:30	**ICTP**
12:00-12:30	A. Vantomme	11:20-12:00	K. Suenaga	11:20-12:00	J. Kotakoski	11:20-12:00	G.-D. Lee		**Colloquium**
12:30-13:00	M. Scardamaglia	12:00-12:40	V. Meunier	12:00-12:40	P. Bøggild	12:00-12:20	M. Edmonds		V. Vuletić
		12:40-13:00	M. Pizzochero	12:40-13:00	R. Niyazov	12:20-12:40	J. Yu		
						12:40-13:00	J. Strand		
13:00-15:00	Lunch	13:00-15:00	Lunch	13:00-14:00	Lunch	13:00-15:00	Lunch	13:00-13:30	Lunch
									Departure
chair:	*A .Krasheninnikov*	*chair:*	*J. Neugebauer*	14:00-	Excursion / Dinner	*chair:*	*D. Golberg*		
15:00-15:40	T. Michely	15:00-15:40	A. Jorio			15:00-15:40	U. Bangert		
15:40-16:20	J. Neugebauer	15:40-16:20	C. Jin			15:40-16:00	M.Tripathi		
		16:20-16:40	S.Kretschmer			16:00-16:20	A. Novikav		
16:20-17:00	Coffee break	16:40-17:00	M. Taherinejad			16:20-17:00	Coffee break		
chair:	*D. Efremov*	17:00-20:00	POSTERS and snacks/beer			*chair:*	*K. Kaasbjerg*		
17:00-17:40	L. Pizzagalli					17:00-17:40	D. Efremov		
17:40-18:20	G. Astakhov					17:40-18:00	V. Carnevali		
18:20-18:40	D. Kvashnin					18:00-18:20	E. Kogan		
19:30-21:30	Welcome Reception					18:20-18:40	D. Fil		