HL 14: 2D Materials: Session II (joint session DS/CPP/HL)

Time: Tuesday 9:30–13:15 Location: H 2032

HL 14.1 Tue 9:30 H 2032

Structural and electronic interactions in vdW heterostructure MoSe2/few-layer-graphene — •Minh Tuan Dau[1], Maxime Gay[1], Daniela Di Felice[2], Céline Vergnaud[1], Alain Marty[1], Cyrille Beigné[1], Gilles Renaud[1], Olivier Renault[1], Pierre Mallet[3], Toai Le-Quang[3], Jean-Yves Veuillen[3], Loïc Huder[1], Vincent Renard[1], Claude Chapelier[1], Giovanni Zamborlini[4], Matteo Jugovac[4], Vitaliy Feyer[4], Yannick Dapp[2], Pascal Pochet[1], and Matthieu Jamet[1] — [1]INAC-SPINTEC-PHELIQS-MEM, LETI, CEA/CNRS, Univ. Grenoble Alpes, F-38000 Grenoble, France — [2]SPEC, CEA, CNRS, Univ. Paris Saclay, CEA Saclay, 91191 Gif-sur-Yvette cedex, France — [3]Institut Néel, CNRS, Univ. Grenoble Alpes, F-38000 Grenoble, France — [4]Peter Grünberg Institute (PGI-6), Forschungszentrum Jülich GmbH, D-52425, Jülich, Germany

We have employed surface-sensitive techniques ranging from atomic resolution (STM-STS) to microscopic scale (synchrotron diffraction, photoemission electron microscopy k-PEEM) in order to probe structural and electronic properties of the van der Waals (vdW) heterojuction: MoSe2/few-layer-graphene grown by molecular beam epitaxy. We find that the crystallographic directions of the MoSe2 lattice align perfectly along the ones of graphene, resulting in only one commensurate configuration. Furthermore, we observe a clear evolution of the band structure of the heterojunction compared to the one of bare few-layer-graphene. Indeed, we evidence a large bandgap opening in few-layer-graphene resulting from significant charge transfer between vdW layers.

HL 14.2 Tue 9:45 H 2032

Interplay of magnetization between graphene and magnetoelectric multiferroics — •Zeila Zanolli — RWTH Aachen Uiniversity, Aachen, Germany

Graphene and magnetoelectric multiferroics are promising materials for spintronic devices with high performance and low energy consumption. We combine the features of both materials by investigating from first principles the interface between graphene and $BaMnO_3$, a magnetoelectric multiferroic. We show [1] that the hybrid systems behaves as a spin filter. Electron charge is transferred across the interface and magnetization is induced in the graphene sheet due to the strong interaction between C and Mn. A remarkably large proximity induced spin splitting of the Dirac cones (300 meV) is achieved and doping can make the high-mobility region of the electronic bands experimentally accessible.

Going further, we investigate spin dynamics at finite temperature using a Monte Carlo approach with exchange coupling parameters fitted from first principles. We find that graphene strongly affects the magnetic properties of the substrate, beyond the interface layer, and induces a softening of the Mn magnetization.

Spin Orbit Coupling calculations reveal that the influence of graphene on the substrate is even more radical and is able to change the direction of the easy axis with respect to the bare $BaMnO_3$ surface. We predict a Rashba splitting of the electronic bands near the K point, and the presence of a Quantum Anomalous Hall effect.

[1] Z. Zanolli, Sci. Rep., 6 (2016) 31346

HL 14.3 Tue 10:00 H 2032

Gate-Dependent Vacancy Migration in Graphene — •Rohit Babar[1] and Mukul Kabir[1,2] — [1]Department of Physics, Indian Institute of Science Education and Research, Pune, India — [2]Center for Energy Science, Indian Institute of Science Education and Research, Pune, India

Graphene based ultrathin devices offer significant advantage due to their high carrier mobility and a gate-tunable carrier density. However, the experimental observations of vacancy diffusion near room-temperature can potentially lead to undesirable void formation and/or edge modification of such devices. Combining transition state theory with first-principles method, we investigate the microscopic vacancy migration mechanism in graphene and its dependence on gate voltage. The intrinsic vacancy diffusion involves a concerted motion of atoms along with an out-of-plane displacement, which is unique to graphene compared with other 2D materials. We further investigate the migration mechanism under gate voltage and find that the activation barrier non-monotonically increases for both electron and hole doping. The trend in activation barrier is explained via collective-phonon stiffening. We estimate a 10^7-fold decrease in vacancy diffusivity at room temperature. Thus, our findings reveal that the graphene-based devices will not degrade further under device operating condition through vacancy migration.

HL 14.4 Tue 10:15 H 2032

Transition between rhombohedral and Bernal stacking in multilayer graphene flakes — •Fabian Rudolf Geisenhof[1], Felix Winterer[1], and Ralf Thomas Weitz[1,2] — [1]Physics of Nanosystems, Physics Department, Ludwig Maximilians Universität München — [2]NanoSystems Initiative Munich (NIM) and Center for NanoScience (CeNS)

Quantum transport in multilayer graphene is interesting in many aspects. For example, it was shown that in ultraclean samples of graphene bilayers [1] and recently also multilayers [2], the exchange interaction leads to a novel phase, who's nature is currently still under debate. At the heart of answering this question is knowledge of the local stacking order during charge transport experiments. Here, we show that the fabrication process has an impact on the structural properties of the flakes. It can lead to the formation of ripples and even to a non-local transition from ABC to ABA stacking. This transformation has been identified by spatially resolved Raman and scattering SNOM measurements, and we discuss possible reasons.

[1] R.T. Weitz, M.T. Allen, B.E. Feldman, J. Martin, and A. Yacoby, "Broken-symmetry states in doubly gated suspended bilayer graphene", Science 330, 812 (2010)

[2] Y. Nam, D.-K. Ki, M. Koshino, E. McCann and A.F Morpurgo, "Interaction-induced insulating state in thick multilayer graphene", 2D Mater. 3 045014 (2016)

HL 14.5 Tue 10:30 H 2032

Chemical vapour growth and delamination of α-MCl3 nanosheets (M = Ru, Mo, Ti) — •Martin Grönke[1,2], Silke Hampel[1], Peer Schmidt[2], Danny Pohflepp[1], Nadine Bronkalla[1], and Bernd Büchner[1] — [1]Leibniz Institute for Solid State and Materials Research, Dresden, Germany — [2]Brandenburg University of Technology Cottbus-Senftenberg, Germany

The two dimensional honeycomb structure of graphene with one monoatomic layer gave an idea to the introduction of other materials with congeneric pattern. Next to carbon based graphene, black phosphorus and binary transition metal chalkogenides, transition metal halides were highly profiled in theory. Among the interest for different materials with strong anisotropic bonding-dependent interactions, resulting frustration effects in honeycomb structures could stabilize new pattern of cooperative magnetic interactions. One candidate to realize a Kitaev Heisenberg (KH) model is the 2D layered honeycomb magnet α-Rutheniumtrichloride (α-RuCl3). Physical properties in nanoscale systems may differ from the respective bulk phase and could even lead to novel physical properties. We herein present to our knowledge the first approach to synthesize phase pure α-RuCl3 crystals on the nanoscale on a substrate via chemical vapour transport (CVT). Beyond that we reveal capabilities to generate thin 2D structures of isostructural compounds like α-MoCl3 and α-TiCl3 on a suitable substrate by means of CVT. Furthermore we show how to increase the number of nanosheets on as grown substrates by different delamination techniques.

HL 14.6 Tue 10:45 H 2032

Suppression of excitonic absorption in few-layer GaSe — •Arne Budweg[1], Dinesh Yadav[1,2], Alexander Grupp[1], Alfred Leitenstorfer[1], Maxim Trushin[1,3], Fabian Pauly[1,2], and Daniele Brida[1] — [1]Department of Physics and Center for Applied Photonics, University of Konstanz, D-78457 Konstanz, Germany — [2]Okinawa Institute of Science and Technology Graduate University, Onna-son, Okinawa 904-0395, Japan — [3]Centre for Advanced 2D Materials, National University of Singapore, 6 Science Drive 2, Singapore 117546

We study the thickness dependent optical absorption of GaSe via highly sensitive differential transmission measurements. Controlling the number of individual layers in a GaSe nanosheet, we observe a suppression of the excitonic transition below a critical value of 8. Ab-

initio modelling enables us to attribute this behavior to a fundamental change in the band structure which, in thin GaSe, leads to a valence band shaped as an inverted Mexican hat. The observed modulation of the optical properties is intrinsic and does not require control via external parameters like substrate material or an applied electric field. Therefore GaSe provides attractive resources for the development of functional optoelectronic devices based on a single material.

HL 14.7 Tue 11:00 H 2032

Lateral heterostructures for sensing small molecules: electronic current features — Ganesh Sivaraman[1], Frank C. Maier[1], Fabio A.L. de Souza[2], Rodrigo G. Amorim[3], Wanderla L. Scopel[2], Ralph H. Scheicher[4], and •Maria Fyta[1] — [1]Institute for Computational Physics, University of Stuttgart, Germany — [2]Departamento de Fisica, Univer- sidade Federal do Espirito Santo, Brazil — [3]Universidade Federal Fluminense, Departamento de Física, Volta Redonda/RJ, Brazil — [4]Department of Physics and Astronomy, Materials Theory, Uppsala University, SwedenDe

Using density functional theory based calculations with the non-equilibrium Greens functions approach, we study in detail the structural, transport, and electronic properties of two types of lateral 2D heterostructures. The first is a combination of graphene with hexagonal boron-nitride (G/hBN). The second is a (1T) metallic MoS_2 phase embedded in a (2H) semiconducting MoS_2 phase (1T/2HMoS_2). Our results identify the importance of the interface within these materials and provide the relation to the electronic current flowing across these. Having understood the basic properties of these structures, we further reveal their high potential and relevance in detecting small molecules. On one hand, we show that the G/hBN heterostructure can detect small gas molecules. On the other hand, by opening a small pore in the 1T/2HMoS_2 heterostructure, we can distinguish between DNA nucleotides. Proof of both detection schemes is provided through the distinct electronic properties and the clear electronic current signals for the various molecules and each heterostructure.

15 min. break

HL 14.8 Tue 11:30 H 2032

Thickness dependent electronic and optical properties of TMDCs within many-body perturbation theory — •Philipp Marauhn, Peter Krüger, and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany

Experimental studies have shown that the spectrum of MoS_2 and other TMDC materials strongly depends on the number of layers of the system. With increasing thickness of a system, the optical absorption spectrum is generally shifted to lower energies.

In this talk we address this behaviour from a theoretical point of view. To investigate the excited electronic states of the TMDCs, we perform three consecutive steps: (i) DFT (ii) *GW* (iii) BSE (Bethe-Salpeter equation). Our results show that both the fundamental quasiparticle gap and the exciton binding energy are significantly reduced when the number of layers is increased. These two effects do not perfectly compensate each other, but lead to an effective shift of the excitation energies towards lower energy. This redshift with increasing number of layers is in agreement with experimental differential reflectance measurements [1]. We also find significant changes in the wave function of some exciton resonances with increasing sample thickness. In multilayer systems, excitons may be composed from electrons and holes situated on different layers, which can be considered as interlayer excitons [2].

[1] Y. Niu et. al., submitted
[2] A. Arora et. al., Nat. Commun., 8(1), 639 (2017)

HL 14.9 Tue 11:45 H 2032

Elasticity theory for two dimensional systems at finite temperatures — •Johannes Häring and Matthias Fuchs — FB Physik, Universität Konstanz, 78457 Konstanz, Germany

According to the Mermin-Wagner theorem many two dimensional systems only exhibit quasi-long-range order. Recently, we developed an elasticity theory for crystals with point defects and applied it to the defect rich cluster crystal [1]. The theory is able to handle long-range translational order. Now we present a method which includes quasi-long-range order.

Furthermore, orientational degrees of freedom are considered as well. As an example results of the helicity modulus and dynamical matrix of the two dimensional XY model are presented. Temperatures range between zero and the Kosterlitz-Thouless transition.

Finally, the influence of topological defects like vortices is discussed.

[1] J.M. Häring, C. Walz, G. Szamel, and M. Fuchs, Phys. Rev. B **92**, 184103 (2015)

HL 14.10 Tue 12:00 H 2032

Ab Initio Study of the Electronic and Optical Properties of Organic-Inorganic two-dimensional Perovskites: The Role of Many-Body Effects — •Maurizia Palummo[1] and Giacomo Giorgi[2] — [1]INFN and Dip. Fisica University of Roma "Tor Vergata" Via della ricerca scientifica 1 Rome Italy — [2]Dip. Ing. Civile e ambientale Univ. Perugia Italy

Organic-Inorganic Halide Perovskites (OIHPs) represent the most relevant breakthrough in the last decade in photovoltaics (PV) Despite the many attractive features, some serious issues remain that prevent their usage in device mass production, such as the fast air/moisture induced degradatio. For this reason, in the last years two-dimensional Ruddlesden-Popper perovskites (2D-RPOIHPs) have emerged as an alternative to 3D bulk for their superior photo- and chemical-stability coupled with high-performance opto-electronic properties and an enhanced hydrophobic nature of the organic part. While the experimental interest towards this 2D class of materials is nowadays well assessed, ab-initio studies focusing on the role of many-body effects are very limited. By means of a coupled GW plus BSE approach on top of DFT-KS simulations, we here study the electronic and optical properties of a 2D-RPOIHP, as a single sheet and also as a periodic QW. A giant band-gap renormalization of the electronic band-gap and the formation of a strongly bound almost 2D excitons are observed. The relationship between the number of layers is discussed.

HL 14.11 Tue 12:15 H 2032

Layered van der Waals crystals with hyperbolic light dispersion — •Morten Gjerding — DTU Physics, Fysikvej building 311, 2800 Kgs. Lyngby

Compared to artificially structured hyperbolic metamaterials, whose performance is limited by the finite size of the metallic components, the sparse number of naturally hyperbolic materials recently discovered are promising candidates for the next generation of hyperbolic materials. Using first-principles calculations, we extend the number of known naturally hyperbolic materials to the broad class of layered transition metal dichalcogenides (TMDs). The diverse electronic properties of the transition metal dichalcogenides result in a large variation of the hyperbolic frequency regimes ranging from the near-infrared to the ultraviolet. Combined with the emerging field of van der Waals heterostructuring, we demonstrate how the hyperbolic properties can be further controlled by stacking different two-dimensional crystals opening new perspectives for atomic-scale design of photonic metamaterials. As an application, we identify candidates for Purcell factor control of emission from diamond nitrogen-vacancy centers.

HL 14.12 Tue 12:30 H 2032

Influence of Hansen solubility parameters on a shear exfoliation process of organophilic layered silica in chloroform — •Michael Huth, Jonas Köhling, and Veit Wagner — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Nanocomposites based on layered silica can be used for several applications, like reinforcement, flame retardant agent, or barrier applications. The understanding of delamination processes of layered silica in organic solvents/polymers is a critical step towards preparing such nanocomposites. In this work, layered silicas with different intercalated molecules are used. Those molecules change the silica surface interaction energies described by Hansen solubility parameters (HSP). HSP of four different synthetic organophilic layered silicas are determined. This allows calculating the dispersibility in chloroform via the Flory-Huggins (F-H) parameter. The F-H parameter can predict the delamination state of organophilic layered silicas in solvents. The delamination state is evaluated quantitatively using atomic force microscopy (AFM). In the case of a high F-H parameter ($\chi > 0.15$), aggregated and unstable layered silica dispersions are found. Whereas in the case of F-H parameters near zero, exfoliated and stable layered silica dispersions are obtained. Additionally, the presence of the surfactant on the surface of fluoromica flakes after exfoliation is proven by Fourier-transform infrared spectroscopy (FT-IR), and density functional theory (DFT) calculations.

HL 14.13 Tue 12:45 H 2032

Theoretical description of photoemission spectroscopy of van der Waals structures — •Bruno Amorim — CeFEMA, Instituto Superior Técnico, University of Lisbon, Av. Rovisco Pais, PT-1049-001 Lisboa, Portugal

I present a general theory to model the angle resolved photoemission spectroscopy (ARPES) of van der Waals (vdW) structures. VdW structures are formed by lattice mismatched and/or misaligned stacked layers of two-dimensional materials and can be commensurate or incommensurate.

The present theory is based on a tight-binding description of the bound electrons and the concept of generalized umklapp processes, being capable of describing both commensurate and incommensurate structures for arbitrary lattice mismatch/misalignment. In this way, the present theory goes beyond previous descriptions of ARPES in incommensurate vdW structures, which are based on continuous, low energy models, which limits their applicability to structures with small lattice mismatch/misalignment.

As an example, I apply the general method to the case of twisted bilayer graphene, obtaining the ARPES bands and ARPES constant energy maps.

The present theory should be useful in correctly interpreting experimental results of ARPES of vdW structures and other system displaying competition between different periodicities, such as density wave phases.

HL 14.14 Tue 13:00 H 2032

Manipulating the Mechanical Properties of Ti2C MXene: Effect of Substitutional Doping — •Poulami Chakraborty[1], Tilak Das[2], Dhani Nafday[1], Lilia Boeri[3], and Tanusri Saha-Dasgupta[1] — [1]Department of Condensed Matter Physics and Materials Science, S.N.Bose National Centre for Basic Sciences, JD Block, Sector-3, Salt Lake , Kolkata 700106, India — [2]Department of Physical Sciences, Indian Institute of Science Education and Research-Kolkata, Mohanpur Campus, PO BCKV Campus Main Office, Nadia * 741252, West Bengal, India — [3]Institute for Theoretical and Computational Physics, TU Graz, Petersgasse 16, 8010 Graz, Austria

Two-dimensional transition metal carbides/nitrides $M_{n+1}X_n$ termed as MXenes have attracted immense interest as potential candidates for Li-ion battery anodes and as a hydrogen storage medium. Our work focuses on the specific case of Ti_2C and Ti_2CO_2 under various tensile strain using density functional theory (DFT). We consider substitutional doping of B and V at Ti and C sites of Ti_2C. We have studied substitutional doping with no surface termination as well as oxygen terminated Ti_2C, i.e., Ti_2CO_2. In-plane stiffness, Young's modulus, and critical strain calculations conclude that B doping is highly effective in improving the elastic properties. This trend is found to hold good even for B-doped and V-doped O terminated systems. However the O passivated compounds are found to have relatively higher critical strain values compared to their pristine counterparts. Thus B doped Ti_2CO_2 , $Ti_2(C_{0.5}, B_{0.5})O_2$, appears to be the best candidate among the studied systems, as compared to pure Ti_2C.