O 105: 2D Materials VII: Heterostructures (joint session O/TT)

Time: Friday 10:30–12:45 Location: MA 005

O 105.1 Fri 10:30 MA 005

Defect-free two-dimensional core-shell heterostructures: MoS_2-TaS_2/Au(111) — Kai Mehlich[1,2], Mahdi Ghorbani-Asl[3], Daniel Sahm[4], Thais Chagas[4], Daniel Weber[1], Catherine Grover[1], Daniela Dombrowski[1,2], Arkady Krasheninnikov[3], and •Carsten Busse[1,2] — [1]Department Physik, Universität Siegen, Germany — [2]Institut für Materialphysik, Universität Münster, Germany — [3]Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Germany — [4]Department Bauingenieurwesen, Universität Siegen, Germany

We prepared two-dimensional core-shell heterostructures of the monolayer transition metal dichalcogenides (TMDCs) MoS_2 and TaS_2 by reactive molecular beam epitaxy (MBE) on chemically inert and weakly interacting Au(111). The heterostructures are in a size regime where quantum confinement can be expected. Despite large lattice mismatch a seamless interconnection of the two materials has been achieved, confirming successful encapsulation of the semiconducting core by a metallic shell. The resulting strain is analyzed on the atomic scale using scanning tunneling microscopy (STM) and compared to continuum models as well as simulations unsing empirical potentials.

O 105.2 Fri 10:45 MA 005

Growth and nanomanipulation of ultrathin Bismuthene nanoflakes on h-BN monolayers — •Antonio J. Martínez-Galera[1,2,3] and José M. Gómez-Rodríguez[2,3,4] — [1]Departamento de Física de Materiales, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [2]Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [3]Instituto de Ciencia de Materiales Nicolás Cabrera, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [4]Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain

Bismuthene, a young member of the family of 2D Materials, exhibits unique electronic properties when reduced to a single layer [1,2]. This study explores the growth of thin bismuth nanoflakes on h-BN monolayers under ultrahigh vacuum conditions. High-resolution scanning tunneling microscopy (STM) images unveil a stacking arrangement of Bi atoms within the nanoflakes, similar to the structure of Bi(110) planes in bulk material. Precise control of nanoflakes thickness, down to the lower limit of a bilayer, has been achieved by adjusting the deposited Bi amount on the h-BN surfaces. In addition to the structural characterization, well-controlled nanomanipulation experiments by using the STM tip have been conducted with these nanoflakes.

References:
[1] F. Reis et al. Science 357, 287-290 (2017).
[2] S. Zhang et al. Chem. Soc. Rev. 47, 982-1021 (2018).

O 105.3 Fri 11:00 MA 005

Optical properties of van der Waals TMD heterostructures from first-principles — •Riccardo Reho[1,2] and Zeila Zanolli[1,2] — [1]Chemistry Dept., Debye Institute for Nanomaterials Science, Utrecht University, Utrecht, The Netherlands — [2]ETSF

Van der Waals (VdW) heterostructures of two-dimensional transition metal dichalcogenides (TMDs) provide a unique platform to investigate rich phenomena stemming from the intricate interactions of charge, spin, and moiré superlattice with many-body effects. Controlling and predicting their optical properties with precision remains challenging.

Employing the ab initio GW-BSE method, we will offer an in-depth microscopic description of the optical properties of TMDs heterostructures. Beyond conventional electronic and absorption analyses, we also delve into the Photoluminescence spectra, leveraging a recent implementation we introduced in the Yambo code. We discuss on the roles of various degrees of freedom, such as mechanical strain and twist alignment. Our findings underscore the importance of structural properties, especially geometrical relaxation and computational subtleties, in ensuring accurate predictions of the band structure and absorption spectra for MoS_2/WS_2 and $MoSe_2/WSe_2$ heterostructures. Notably, we report a pronounced excitonic shift attributed to twisting and strain, shedding light on their profound impact on optical properties.

O 105.4 Fri 11:15 MA 005

Complexity of excitons at the TMD-Graphene interface — •Amir Kleiner, Daniel Hernangómez Pérez, and Sivan Refaely-Abramson — Weizmann Institute of Science, Rehovot, Israel

The complex optical characteristics of heterostructures composed of layered 2D materials are of great importance and interest. Specifically, the interaction between light and matter at the interface of layered transition metal dichalcogenides (TMDs) and graphene draw significant interest, facilitating the understanding of related energy-transfer mechanisms and their structural roots. We use state-of-the-art first principles calculations to study the dependence of the excitonic composition and absorption properties of the representative WS_2 - Graphene heterostructures on the structural details of these structures. Examining the cases of 0° and 30° degrees of interlayer twist angle, we find that the induced Brillouin zone mismatch, and concomitantly the energy level alignment between the graphene Dirac cone and the TMD bands, dictate the excitonic properties resulting in significant variation between the two systems. In particular, these set the charge-separation of nature of low-energy interlayer excitons and the state hybridization of optically active intralayer excitonic peaks. We use our results to numerically quantify the graphene-induced homogeneous broadening as a function of heterostructure alignment. Our findings provide guidelines for optical excitations based on the composition of the heterostructure, indicating a direct connection between the stacking of the layers, the separation of charges within the excitons, and the broadening of optical features.

O 105.5 Fri 11:30 MA 005

Electronic Characterization of Magnetic $CrCl_3$ Monolayers on $NbSe_2$ — •Jan Cuperus, Anna Reinhold, Daniel Vanmaekelbergh, and Ingmar Swart — Debye Institute for Nanomaterials Science, Utrecht University, The Netherlands

Electronic devices today suffer from a considerable loss of energy in the form of heat. With the ever increasing scale of information processing, it is essential to develop devices that are more efficient either in power usage or in information processing. In both cases, new materials are required to enable this. Van der Waals heterostructures are a class of materials that are well suited to offer the required properties. By combining materials with different properties in a heterostructure with a high quality interface, a plethora of properties can be obtained. Recently, this strategy was used to obtain topological superconductivity by combining superconducting $NbSe_2$ with ferromagnetic $CrBr_3$ [1].

We have conducted STM experiments on a similar heterostructure, replacing the out-of-plane ferromagnetism of CrBr3 by the in-plane ferromagnetism of $CrCl_3$. We present the MBE growth of $CrCl_3$ on $NbSe_2$ and structural insight into the formed heterostructure by STM measurements. In addition, the electronic structure is investigated using differential conductance measurements, both with and without an externally applied magnetic field. We show that the superconductivity of $NbSe_2$ couples to the in-plane ferromagnet, thereby introducing in-gap states.

[1] S. Kezilebieke, et al. Nature 588, 424-428 (2020).

O 105.6 Fri 11:45 MA 005

Interplay of tunnelling gap and Faraday-like screening in graphene heterostructures — •Tobias Wichmann[1,2,3], Keda Jin[1,2,4], Jose Martinez Castro[1,4], Honey Boban[5], Lukasz Plucinski[5], Tom G. Saunderson[6,7], Yuriy Mokrousov[6,7], Markus Ternes[1,2,4], F. Stefan Tautz[1,2,3], and Felix Lüpke[1,2] — [1]Peter-Grünberg-Institut (PGI-3), Forschungszentrum Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA) - Fundamentals of Future Information Technology, Germany — [3]Institut für Experimentalphysik IV A, RWTH Aachen, Germany — [4]Institut für Experimentalphysik II B, RWTH Aachen, Germany — [5]Peter-Grünberg-Institut (PGI-6), Forschungszentrum Jülich, Germany — [6]Institute of Physics, Johannes Gutenberg University, Mainz, Germany — [7]Peter-Grünberg-Institut (PGI-1) and Institute for Advanced Simulations (IAS), Forschungszentrum Jülich, Germany

Scanning tunneling spectroscopy of graphene shows a gap around the Fermi energy, as tunnelling channels to the graphene Dirac states are suppressed due to their finite momentum in the graphene plane. Until now, applications of this phenomenon have been lacking. We report the interplay of the tunnelling gap and Faraday-like screening in graphene placed on Fe_3GeTe_2 (FGT). By tunnelling through the electronic gap

of the graphene into the underlying FGT surface, we directly access the electronic properties of the graphene/FGT van der Waals interface. Studying the magnetoelectric tunability of the heterostructure properties, we find Faraday-like screening of the electric field exerted by the tunnelling probe by the graphene.

O 105.7 Fri 12:00 MA 005

Probing the phase transition to a coherent 2D kondo lattice — •Cosme Gonzalez Ayani[1,2,3], Michele Pisarra[4], Ivan M. Ibarburu[2,3], Manuela Garnica[2], Rodolfo Miranda[2,3,5], Fabian Calleja[2], Fernando Martin[2,3], and Amadeo L. Vazquez de Parga[2,3,5] — [1]Institute of Physics, Zagreb, Croatia — [2]Universidad autonoma madrid, Madrid, Spain — [3]Imdea Nanociencia, Madrid, Spain — [4]Universita della Calabria, Rende, Italy — [5]IFIMAC, Madrid, Spain

Kondo screening occurs when a magnetic impurity is embedded in a metal, below a given temperature, known as the Kondo temperature, a singlet state forms between the spin of the impurity and the spins of the conduction electrons. When the distance between the magnetic impurities is small enough the physics of the system is expected to be modified. The first experimental evidence was obtained in the 1970s in systems containing rare earths. By means of scanning tunneling microscopy (STM) and spectroscopy (STS) at low temperatures we explore a van der Waals heterostructure consisting in a single layer of 1T-TaS2 on a 2H-TaS2 crystal. The 1T-TaS2 layer presents a (13x13)R13.9 charge density wave (CDW) with a localized electron at the center of every unit cell of the CDW. For temperatures below 28 K the spatially resolved STS shows the presence of a Kondo resonance in the Mott-Hubbard gap. For temperatures below 11 K the system develops a quantum coherent state called Kondo lattice, resembling the physics of 3D heavy fermion metals.

O 105.8 Fri 12:15 MA 005

Engineering quantum dot nanoarrays in van der Waals heterostructures — •Keda Jin[1,2], Lennart Klebl[3], Junting Zhao[1,2], Tobias Wichmann[1,5], F. Stefan Tautz[1,5], Felix Lüpke[1], Dante Kennes[4], Jose Martinez-Castro[1,2], and Markus Ternes[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Institut für Experimentalphysik II B, RWTH Aachen, 52074 Aachen, Germany — [3]I.Institute for Theoretical Physics, Universität Hamburg, 22607 Hamburg, Germany — [4]Institut für Theorie der statistischen Physik, RWTH Aachen, 52074 Aachen — [5]Institut für Experimentalphysik IV A, RWTH Aachen, 52074 Aachen, Germany

Superlattice engineering in graphene has generated interest for their ability to mimic the moiré potential observed in twistronics. While the moiré potential is sensitive to the twist angle, we present a method to periodically modulate the graphene potential by stacking graphene on 1T/2H-$NbSe_2$. The doping effect from the charge density wave of 1T-$NbSe_2$ allows for the formation of quantum dot nanoarrays. Using scanning tunneling microscopy/spectroscopy, we visualized the localized electronic structures to be independent of the twist angle between graphene and $NbSe_2$. Furthermore, we observed a bias-dependent strip pattern, breaking the six-fold rotational symmetry, which indicates an emergence of correlated states in the quantum dot nanoarrays. Our research paves the way for the fabrication of quantum dot nanoarrays in van der Waals heterostructures, extending beyond graphene to other 2D van der Waals heterostructures that are not limited by twist angle.

O 105.9 Fri 12:30 MA 005

Mechanical Characterization of Molecular Sieving Polymers — •Jakob Kreie[1], André Beyer[1], Yonghang Yang[2], Zhikun Zheng[2], and Armin Gölzhäuser[1] — [1]Physics of Supramolecular Systems and Surfaces, Bielefeld University, Germany — [2]School of Chemistry, Sun Yat-sen University, Guangzhou, Guangdong, Republic of China

To enable the practical use of molecular sieves on a larger scale, it is crucial to achieve a certain mechanical stability and elasticity. Our study deals with the analysis of polymer membranes as molecular sieves, these 2D imine-linked covalent organic frameworks are periodic and porous networks. The focus of the research is on their permeability as well as their mechanical properties.

Through the application of an atomic force microscope, we conducted comprehensive evaluations using free-standing nanoindentation and the bulge test. The results revealed a Young's modulus of 55 GPa and a breaking strength of 83 N/m for a membrane thickness of 45 nm. Moreover, our observations demonstrated remarkable elasticity during repeated tests, even after localized damage to the free-standing membrane had occurred.