DS 5: 2D Materials and their Heterostructures II: Graphene and Graphene Containing Heterostructures

Time: Tuesday 9:30–11:45 Location: A 053

DS 5.1 Tue 9:30 A 053

Strain-modulated defect engineering of two-dimensional materials — •Prosun Santra[1], Sadegh Ghaderzadeh[2], Mahdi Ghorbani-Asl[1], Hannu-Pekka Komsa[3], Elena Besley[2], and Arkady Krasheninnikov[1] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany. — [2]School of Chemistry, University of Nottingham, Nottingham, U.K. — [3]Microelectronics Research Unit, University of Oulu, Oulu, Finland.

We have studied the response to external strain of h-BN, graphene, $MoSe_2$, and phosphorene, four archetypal 2D materials, which contain substitutional impurities, using first-principles calculations. We find that the formation energy of the defect structures can either increase or decrease with bi-axial tensile strain, depending on the atomic radius of the impurity atom which can be larger or smaller than that of the host atom. Analysis of the strain maps indicates that this behavior is associated with the compressive or tensile local strains produced by the impurities that interfere with the external strain. The discovered trends are consistent across all studied 2D materials and are likely to be general. Our findings open up opportunities for combined strain- and defect-engineering to tailor the opto-electronic properties of 2D materials, and specifically, the location and properties of single-photon emitters.

DS 5.2 Tue 9:45 A 053

Twist angle dependent proximity induced spin-orbit-coupling in graphene/NbSe2 heterostructures — •Thomas Naimer[1], Martin Gmitra[2], and Jaroslav Fabian[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Pavol Jozef Safarik University in Kosice, 04001 Kosice, Slovakia

We investigate the effect of the twist angle on the proximity spin-orbit coupling (SOC) in graphene/niobium diselenide (Gr/NbSe2) heterostructures from first principles. The low energy Dirac cones of several different commensurate twisted supercells are fitted to a model Hamiltonian, allowing us to analyze the twist-angle dependency of the SOC in detail. This reveals the possibility to triple the Rashba SOC, when going from 0° to 30° twist angle. Furthermore, at a critical twist angle of 23° the in-plane spin structure acquires a significant radial component, enabling collinear charge-to-spin conversion. Analyzing the Dirac cone with respect to allowed Umklapp processes and orbital decomposition shines light on the observed twist angle dependencies. In addition, we evaluate the potential for (collinear and perpendicular) charge-to-spin conversion in such heterostructures within linear response theory. This work was funded by the Elite Network of Bavaria, the Deutsche Forschungsgemeinschaft (DFG), SFB 1277, SPP 2244 and by the European Union Horizon 2020 Research and Innovation Program under contract number 881603 (Graphene Flagship). M.G. acknowledges VEGA 1/0105/20.

DS 5.3 Tue 10:00 A 053

Ultra-sensitive real-time detection of SARS-CoV-2 proteins with carbon nanomembrane/graphene field-effect transistor heterostructure — •Hamid Reza Rasouli[1], David Kaiser[1], Ghazaleh Eshaghi[1], Marco Reinhard[2], Alexander Rolapp[2], Dominik Gary[3], Katrin Frankenfeld[3], Thomas Weimann[4], Michael Meister[2], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena, Germany — [2]Institut für Mikroelektronik- und Mechatronik-Systeme gemeinnützige (IMMS GmbH), 99099 Erfurt, Germany — [3]Forschungszentrum für Medizintechnik und Biotechnologie (fzmb GmbH), 99947 Bad Langensalza, Germany — [4]Physikalisch-Technische Bundesanstalt (PTB), 38116 Braunschweig, Germany

This study presents a novel approach to detect SARS-CoV-2 proteins based on graphene field effect transistors (GFET) functionalized via the van der Waals assembly with carbon nanomembranes (N3-CNM) enabling immobilization of antibodies for specific detection of the S- and N-proteins. A distinctive aspect of this approach is the simultaneous measurements of 15 GFETs integrated on a single chip with an automatic microfluidic system, facilitating the reliability for measuring the binding responses. The results demonstrate a detection limit down to the attomolar range with a dynamic response of 5 orders of magnitude. Furthermore, successful multiplex detection of S-protein and N-protein is demonstrated. The presented methodology paves the way towards highly sensitive, rapid, specific and multiplex detection of targets in various antibody-antigen systems.

DS 5.4 Tue 10:15 A 053

Graphene meets the macroscopic world: structure-property relationships and intercalation — •Florian Fuchs[1,2,3], Fabian Teichert[1,2,3], Daniel Dick[1,2,3], and Jörg Schuster[1,2,3] — [1]Center for Microtechnologies, Chemnitz University of Technology, Chemnitz, Germany — [2]Fraunhofer Insitute for Electronic Nano Systems (ENAS), Chemnitz, Germany — [3]Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology, Chemnitz, Germany

We study graphene-based conductor materials to leverage the excellent electronic transport properties of graphene into the macroscopic world. In these conductor materials, the individual graphene flakes form a layered macrostructure. A network model has been developed to relate microscopic graphene flake properties to the resulting macroscopic transport properties. Different flake sizes, packing densities, and contact geometries can be studied with this approach.

In addition, the layered structure of graphene-based conductor materials enables further material tuning by intercalating suitable materials in-between the graphene layers. An overview over different ongoing investigations of such systems, which are driven forward by density functional theory, will be given. We discuss the impact of different intercalants, like metal atoms and small molecules, onto the structural and electronical properties.

15 min. break

DS 5.5 Tue 10:45 A 053

Spin injection and detection in fully two-dimensional van der Waals devices — •Jan Bärenfänger[1], Kenji Watanabe[2], Takashi Taniguchi[2], Jonathan Eroms[1], Dieter Weiss[1], and Mariusz Ciorga[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Deutschland — [2]National Institute for Materials Science, Tsukuba, Japan

In recent years, two-dimensional (2D) materials have attracted considerable attention for spintronic applications due to their vast electrical and magnetic properties. Especially, graphene, with its long spin relaxation times, and ferromagnetic Fe_3GeTe_2 (FGT), with its sharp magnetic switching behaviour and Curie temperatures up to room temperature, are 2D materials that seem to be predestined for spintronic applications. In this work we report efficient out-of-plane spin injection and detection in an all 2D van der Waals heterostructure using only exfoliated 2D materials. We demonstrate the spin-valve and Hanle effects in the non-local transport configuration in a stack of FGT, hexagonal boron nitride (hBN) and graphene layers. FGT flakes form the spin-aligning electrodes necessary to inject spins into the graphene channel and subsequently detect them. The hBN tunnel barrier provides a high quality interface between the ferromagnetic electrodes and graphene, eliminating the conductivity mismatch problem, thus ensuring efficient spin injection and detection. Our results demonstrate that FGT/hBN/graphene heterostructures form a promising platform for realizing 2D van der Waals spintronic devices.

DS 5.6 Tue 11:00 A 053

Extended Hubbard model describing small multi-dot arrays in bilayer graphene — •Angelika Knothe[1] and Guido Burkard[2] — [1]Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany — [2]Department of Physics, University of Konstanz, 78457 Konstanz, Germany

Confined quantum dot states are attractive for various applications, from qubits to store quantum information to simulating exotic quantum phases. Here, we set up and parametrize a Hubbard model for interacting quantum dots in bilayer graphene and study double dots as the smallest multi-dot system. We demonstrate the tunability of the spin and valley multiplets, Hubbard parameters, and effective exchange constant by, e.g., gates and a magnetic field. For half-filling and large valley splittings, we derive and parametrize an effective Heisenberg model for the quantum dot spins.

DS 5.7 Tue 11:15 A 053

Spin-Orbit Torque in Graphene / 1T-TaS$_2$ heterostructure — •Maedeh Rassekh[1], Marko Milivojević[2,3], and Martin Gmitra[1,4] — [1]Institute of Physics, Pavol Jozef Šafárik University in Košice, Košice, Slovakia — [2]Institute of Physics, Pavol Jozef Šafárik University in Košice, Košice, Slovakia — [3]Faculty of Physics, University of Belgrade, Belgrade, Serbia — [4]Institute of Experimental Physics, Slovak Academy of Sciences, Košice, Slovakia

Spin-orbit torque (SOT) plays a critical role in enabling low-power and high-speed operation. In this study, we focus on investigating SOT acting on proximity-induced magnetization in graphene for the charge density wave ferromagnetic phase of 1T-TaS$_2$. Our findings reveal that the orientation and strength of the induced magnetization are influenced by the in-plane magnetization within the 1T-TaS$_2$ layer. Notably, alterations in the in-plane magnetization orientation within the 1T-TaS$_2$ layer led to the switching of charge-to-spin conversion mechanisms between the spin Hall effect and the Rashba-Edelstein effect. Furthermore, we extend our investigation to explore the impact of doping, particularly focusing on the vicinity of the Dirac point and hole-doped graphene. Our results highlight the importance of Fermi energy tuning for customizing spin transport properties in graphene/1T-TaS$_2$ heterostructures, which hold significant potential for future technological advancements. This work was supported by the APVV-SK-CZ-RD-21-0114, SASPRO 2 No. 945478, FLAG ERA JTC 2021 2DSOTECH, and IMPULZ IM-2021-42 projects.

DS 5.8 Tue 11:30 A 053

Proximity enhancement of Rashba angle in graphene/1T-TaS$_2$ heterostructures — •Martin Gmitra[1,2], Marko Milivojević[3,4], and Karol Szałowski[5] — [1]Institute of Physics, Pavol Jozef Šafárik University in Košice, 04001 Košice, Slovakia — [2]Institute of Experimental Physics, Slovak Academy of Sciences, 04001 Košice, Slovakia — [3]Institute of Informatics, Slovak Academy of Sciences, 84507 Bratislava, Slovakia — [4]Faculty of Physics, University of Belgrade, 11001 Belgrade, Serbia — [5]University of Łódź, Faculty of Physics and Applied Informatics, Department of Solid State Physics, 90-236 Łódź, Poland

Van der Waals heterostructures provide unprecedented control of Dirac electronic states in graphene via proximity effects. In the talk, we present an electronic structure study of graphene/1T-TaS$_2$ heterostructure and show that the charge density wave phase in 1T-TaS$_2$ monolayer enhances significantly the Rashba angle in proximitized graphene. The Rashba spin-orbit coupling parameters can be further enhanced by applying a transverse electric field. We found also that the particular sandwich structures 1T-TaS$_2$/graphene/1T-TaS$_2$ trigger the Rashba angle to the $\pi/2$ limit relevant for specific charge-to-spin conversion utilizing collinear Rashba-Edelstein effect.

This work was supported by the APVV SK-CZ-RD-21-0114, FLAG ERA JTC 2021 2DSOTECH, IMPULZ IM-2021-42, and SASPRO 2 No. 945478 research grants.