DS 22: 2D Materials 8 (joint session DS/CPP)

Time: Thursday 9:30–11:30 Location: H17

DS 22.1 Thu 9:30 H17

Calculation of Elastic Properties in Monolayer Covalent-Organic Frameworks — •David Bodesheim[1], Antonios Raptakis[1], Jonathan Heinze[1], Arezoo Dianat[1], Robert Biele[1], Alexander Croy[2], and Gianaurelio Cuniberti[1] — [1]TU Dresden, Dresden, Germany — [2]FSU Jena, Jena, Germany

Covalent-Organic Frameworks (COFs) are crystalline porous materials that are based on organic monomeric units, so called building blocks. Through recent experimental progress, mono- and few-layer COF materials have been synthesized, providing a new class of 2D materials.[1,2] From a computational point of view, however, accurately calculating properties of these materials is demanding as their unit cells are usually very big. In this work, we calculate elastic properties for a multitude of 2D COFs in a high-throughput manner. The calculations are based on classical force-fields and are compared with higher level of theory like density functional based tight binding (DFTB). We show how force-fields can be very useful for mechanical property calculation, how their accuracy can be improved, and typical fallacies for 2D COFs. Furthermore, we introduce models to predict mechanical properties from the properties of their monomeric building blocks.[3] This paves the way for accurate multiscale modeling, high-throughput calculations, and materials design with properties on demand.

[1] A. Ortega-Guerrero, et al. ACS Appl. Mater. Interfaces, 13, 22, 26411-26420 (2021).
[3] Z. Wang, et al., Nat. Synth., 1, 69-76 (2022).
[3] A. Raptakis, et al. Nanoscale, 13, 1077 (2021).

DS 22.2 Thu 9:45 H17

Light-Matter Interaction in 2D Polar Metals — •Margaux Lassaunière[1], Wen He[2], Katharina Nisi[1], Shruti Subramanian[3], Siavash Rajabpour[3], Alexander Vera[3], Nathalie Briggs[3], Su Ying Quek[2], Joshua Robinson[3], and Ursula Wurstbauer[1] — [1]Institut of Physics, Münster University, Germany — [2]Department of Physics, National University of Singapore, Singapore — [3]MatSE; Center for 2DLM; ATOMIC; 2D Crystal Consort.; Penn State University, USA

Understanding and controlling the light-matter interaction in thin metal films is of high technological relevance. Here, we study the linear optical response of atomically thin 2D gallium, 2D indium as well as their alloys embedded in half-van der Waals heterostructures by spectroscopic imaging ellipsometry. The thin films are prepared via confinement heteroepitaxy (Chet). In a systematic study of the dielectric functions, we separate free and bound electron contributions to the optical response, with the latter pointing towards the existence of thickness-dependent quantum confinement phenomena and epsilon near zero (ENZ) behaviour [1]. The resonance energies of the observed ENZ behaviour are dependent on the number of atomic metal layers, materials, and alloying [2]. Their tunability makes 2D polar metals attractive for quantum engineered metal films, tunable (quantum-)plasmonics and nano-photonics.

[1] K. Nisi et al. Adv. Mater. 2021, 2104265
[2] S. Rajabpour et al. Adv. Funct. Mater. 2020, 2005977

DS 22.3 Thu 10:00 H17

Layer dependent anisotropic dielectric function of the magnetic semiconductor CrSBr — •Pierre-Maurice Piel[1], Margaux Lassaunière[1], Julian Klein[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, Muenster University, Germany — [2]Department of Materials Science and Engineering, Massachusetts Institute of Technology, USA

The van der Waals (vdW) material CrSBr is a 2D magnetic semiconductor with ferromagnetic ordering within each layer. Adjacent layers, however, are coupled antiferromagnetically. As a vdw semiconductor with a direct band gap, the light matter interaction is determined by strong excitonic resonances that are highly anisotropic in the crystal plane. We experimentally determine the complex dielectric function in the near infrared to visible regime along the two main crystal directions by spectroscopic imaging ellipsometry (SIE) measurements and regression analysis to a multilayer model. Unlike other vdW semiconductors such as MoS2 or WSe2 [1], the rich excitonic signatures in the dielectric function are highly anisotropic and show only minor distinct dependence on the number of layers. Even more striking, we find that the excitonic resonance are better pronounced for multilayer compared to monolayer CrSBr with significantly reduced line-width even at room temperature. [1] Wurstbauer et al. J. Phys. D: Appl. Phys. 50, 173001 (2017).

DS 22.4 Thu 10:15 H17

Tracing the Superconducting Phase Transition in Atomically Thin 2D Polar Gallium by Transport and Spectroscopic Ellipsometry — •Jakob Henz[1], Margaux Lassunière[1], Pierre-Maurice Piel[1], Siavash Rajabpour[2], Alexander Vera[2], Joshua Robinson[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, Muenster University, Germany — [2]MatSE; Center for 2DLM; Atomic; 2D Crystal Consort, PennState University, USA

Half van der Waals 2D polar metals are a novel class of 2D materials, realized by confinement heteroepitaxial growth (CHet). Hereby, metal atoms such as gallium or indium are intercalated between graphene and a silicon carbide substrate. This results in large area, environmentally stable, 2D metals with a bonding gradient in z-direction ranging from covalent over metallic to vdW within only two to three atomic layers. The materials feature interesting properties such as superconductivity[1] and a large plasmonic response in the visible range[2]. 2D gallium is studied by temperature dependent spectroscopic ellipsometry and transport measurements down to below 1K. We extract the dielectric function in the visible to near infrared range with a special focus on signatures across the phase transition from metallic to superconducting behavior unambiguously identified from the abrupt drop in the temperature dependent sheet resistance at the transition temperature T_C of about 3.5 K.

1 S. Rajabpour et al., Adv. Mater. 2104265 (2021)
2 Nisi et al., Adv. Funct. Mater. 2005977, 1-11 (2020)

DS 22.5 Thu 10:30 H17

Epitaxial growth of $Fe_{5-x}GeTe_2$ films with a Curie temperature above 300 K on graphene — Hua Lv[1], Jens Herfort[1], Jürgen Schubert[2], Michael Hanke[1], Manfred Ramsteiner[1], and •Joao Marcelo J. Lopes[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Germany — [2]Peter Grünberg Institut (PGI-9), Forschungszentrum Jülich, Germany

Synthesis of magnetic 2D materials exhibiting transition temperatures at or above 300 K is a crucial step towards the development of ultra-compact spintronic devices. Here, we report our recent progress on epitaxial growth of the 2D ferromagnet $Fe_{5-x}GeTe_2$ via MBE on graphene on SiC(0001). Thin films with a thickness of about 10 nm and different Fe concentrations were studied. Characterization performed with methods such as in-situ RHEED and grazing incidence X-ray diffraction confirmed the formation of epitaxial layers with good crystalline quality. Magneto-transport measurements and SQUID magnetometry were employed to assess the electrical and magnetic properties. They reveal that the MBE-grown $Fe_{5-x}GeTe_2$ exhibits a metallic behavior for all investigated Fe concentrations. In addition, composition-dependent magnetic anisotropies and Curie temperatures (T_C) were deduced. For the Fe content close to 5, a predominant easy out-of-plane orientation and T_C well above 300 K were measured. These results are relevant for the further development of wafer-scale fabrication of magnetic 2D materials aiming at the realization of multifunctional, atomically thin devices.

DS 22.6 Thu 10:45 H17

Antisymmetric magnetoresistance in a Fe_3GeTe_2-Fe_3GeTe_2 van der Waals ferromagnetic homojunction — •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, 93040 Regensburg, Germany — [2]NIMS, 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan

The emergence of novel two-dimensional (2D) magnetic van der Waals (vdW) materials have breathed new life into the field of spintronics. The weak vdW interaction between layers of strong covalent bonds enables the exfoliation of these materials down to monolayers. Furthermore, vdW heterostructures can easily be fabricated by stacking

them on top of each other like LEGO blocks, bringing a platform for novel spintronic devices. Here, we report an antisymmetric magnetoresistance (MR) in an Fe3GeTe2- Fe3GeTe2 (FGT) vdW homojunction. We attribute it to eddy currents emerging at the interface of the antiparallel, perpendicular-to-plane magnetized FGT flakes, due to the different sign of the anomalous Hall effect in both flakes. These eddy currents perturb the measured longitudinal resistance, resulting in the observed antisymmetry. Such an interpretation is supported by the observation of a sign change of the MR when measuring the voltage drop along the opposite edges of the transport channel . This work highlights the potential for new spintronic applications using vdW ferromagnets.

DS 22.7 Thu 11:00 H17

Charge-transfer stabilization, modulation doping, and CDW phase in layered ferecrystal heterostructures — •Fabian Göhler[1], Shrinidhi Ramasubramanian[1], Sanam K. Rajak[1], Niels Rösch[1], Adrian Schütze[1], Susanne Wolff[1], Marisa Choffel[2], Dmitri L. M. Cordova[2], David C. Johnson[2], and Thomas Seyller[1] — [1]Chemitz University of Technology, 09126 Chemnitz, Germany — [2]University of Oregon, Eugene 97403, USA

A virtually unlimited number of metastable, layered heterostructures - called *ferecrystals* due to the non-epitaxial alignment between layers - can be grown via the self-assembly of layered amorphous precursors. [1] In this contribution, we want to highlight recent investigations on the electronic structure and interlayer interactions in several series of compounds using photoemission spectroscopy (PES).

In the Bi-Mo-Se system, the formation of the metallic 1T-polytype of $MoSe_2$ is aided by charge transfer from rock-salt structured BiSe. By systematically stacking BiSe, Bi_2Se_3, and $MoSe_2$, the mechanisms which stabilize these structures can be understood. [2]

Compounds prepared from PbSe and VSe_2 layers show charge transfer between layers as well, allowing to tune transport properties via modulation doping. Additionally, the emergence of a charge density wave in the VSe_2 layers has been reported below 100 K [3], and was investigated by angle-resolved PES.

[1] Esters et al., *Angew. Chem. Int. Ed.* **54**, 1130 (2015).
[2] Göhler et al., *J. Phys. Chem. C* **125**, 9469 (2021).
[3] Cordova et al., *Chem. Mater.* **31**, 8473 (2019).

DS 22.8 Thu 11:15 H17

Impact of opto-electronic measurements on the properties of hexagonal boron nitride as a dielectric — •Jo Bertram[1], Luca Kotewitz[1], Manfred Ersfeld[1], Frank Volmer[1], Kenji Watanabe[2], Takashi Taniguchi[3], Christoph Stampfer[1], and Bernd Beschoten[1] — [1]2nd Institute of Physics and JARA-FIT, RWTH Aachen University, 52074 Aachen, Germany — [2]Research Center for Functional Materials, National Institute for Materials Science, Tsukuba, Japan — [3]International Center for Materials Nanoarchitectonics, National Institute for Materials Science, Tsukuba, Japan

Hexagonal boron nitride (hBN) serves as an atomically flat, insulating substrate for a large variety of 2D heterostructures. However, recent opto-electronic experiments showed that optically triggered leakage currents passing through hBN pose a serious bottleneck for reliable gating of 2D semiconductors [1]. Motivated by these observations, we report on photo-induced charge transport through hBN in graphite-hBN-graphite devices. Furthermore, we examine the impact of illuminating hBN employed as a gate dielectric on the charge carrier density of graphene Hall bar devices. Our results indicate that hBN exhibits optically active electronic states, which partially screen the gate electric field under light illumination. Interestingly, we observe a strong asymmetry of this effect for positive and negative electric fields showing that hBN does not behave as an ideal dielectric within the plate capacitor model especially in opto-electronic experiments.

[1] F. Volmer et al., Phys. Status Solidi RRL 14, 2000298 (2020)