DS 35: 2D Materials and their Heterostructures II (joint session DS/O/HL)

Time: Thursday 9:30–10:45 Location: CHE 89

DS 35.1 Thu 9:30 CHE 89

Longitudinal Nonlinear Spin Sensitive Response in two-dimensional Materials — •Dominik Kreil, Mario Graml, and Helga M. Böhm — Institute of Theoretical Physics, Johannes Kepler University Linz, Altenbergerstr. 69, A-4040 Linz, Austria

Future spin- and valleytronic devices will demand a deeper understanding of electronic systems. [1] With increasing intenstitys of state of the art terahertz lasers linear approximations become more imprecise. Nonlinear plasmonic effects arising from coherent oscillations of free charge carriers in metals or highly doped semiconductors serve to enhance optical processes. The underlying dynamics of electrons (or holes) was successfully treated semi-classically [2] in three-dimensional (3D) nanostructures; quantum expressions for up to the third order of the longitudinal nonlinear polarizabilities of the 3D, 2D and 1D homogeneous electron gases as well as graphene are also known. We here present a general discussion of higher order response functions resulting from time-dependent perturbation theory. Using the random phase approximation as in Ref. [3] we also derive a closed formula for longitudinal nonlinear spin sensitive response functions in arbitrary order. It holds for all the above listed systems and for imbalanced spin- or valley-polarizations. An application to the 2D spin-polarized electron gas with parabolic dispersion and in graphene [4,5] is presented.
References: [1] Vitale et al., Small 14, 1801483 (2018). [2] Krasavinet al., Laser & Photonics Reviews 12, 1700082 (2018). [3] Mikhailov, Phys. Rev. B. 93, 085403 (2016). [4] D. Kreil et al., Phys. Rev. B. 92, 085403 (2015). [5] D. Kreil et al., Lithuanian J. Phys. 59, 35 (2019).

DS 35.2 Thu 9:45 CHE 89

Predicting Exfoliability of MAX Phases into MXenes Using Ab-initio Thermodynamics — •Ali Muhammad Malik, Delwin Perera, Jochen Rohrer, and Karsten Albe — Institut für Materialwissenschaft, Technische Universität Darmstadt, Germany

In recent years, research on 2D MAX-derived MXenes has expanded significantly due to their potential application in energy storage systems, electromagnetic interface shielding, electrocatalysis and gas detection. Almost 40 MAX phases have been predicted to be exfoliable based on force constant calculations and exfoliation energies. However, in experiment only 21 have so far been chemically exfoliated. In this work, we present a descriptor that combines calculated reaction energies and surface stabilities under experimentally relevant conditions. In agreement with experiments, we show that this descriptor is indeed capable of predicting the exfoliability of MXenes from Ti-based MAX phases in HF, whereas Cr-based MAX phases are predicted to decompose into Cr_3C_2 (carbide). We suggest that this descriptor is capable to guide experimental synthesis efforts in particular with respect to the choice of etchant and concentration.

DS 35.3 Thu 10:00 CHE 89

Characterization and Stability of Janus TiXY (X/Y= S, Se, and Te) Monolayers — Aybey Mogulkoc[1], Yesim Mogulkoc[1], Seymur Jahangirov[2], and •Engin Durgun[2] — [1]Department of Physics, Ankara University, 06100, Ankara, Turkey — [2]UNAM and Institute of Materials Science and Nanotechnology, Bilkent University, 06800, Ankara, Turkey

The addition of third element to binary 2D structures can lead to superior properties, hence extensive analyses on the characterization of such systems are required to reveal their full potential. In this study, we examine the structural, mechanical, electronic, thermal, and optical properties of TiXY (X/Y= S, Se, and Te) monolayers by using first-principles techniques. The stability of 1T and 2H-phases are revealed by phonon spectrum analysis and molecular dynamics simulations. Following the investigation of the mechanical response, electronic structures are examined together with partial density of states analysis. While monolayers of 1T-TiXY are found to be semimetals, monolayers of 2H-TiXY are semiconductors with indirect band gap. The optical spectrum is obtained by calculating the imaginary dielectric function and is correlated with the electronic structure. The variation of heat capacity with temperature is investigated and low/high temperature response is shown. Finally, possible structural distortions are also taken into account and charge density wave transition in 1T-TiSeS due to Peierls instability is demonstrated. Our results not only reveal the stable Janus monolayers of TiXY but they also point out these systems as promising candidates for nanoscale applications.

DS 35.4 Thu 10:15 CHE 89

Semiconducting defect-free polymorph of borophene: Peierls distortion in two dimensions — Semran Ipek[2], Aybey Mogulkoc[1], •Seymur Cahangirov[2], and Engin Durgun[2] — [1]Department of Physics, Ankara University, 06100, Ankara, Turkey — [2]UNAM and Institute of Materials Science and Nanotechnology, Bilkent University, 06800, Ankara, Turkey

In contrast to the well-defined lattices of various two-dimensional (2D) systems, the atomic structure of borophene is sensitive to growth conditions and type of the substrate which results in rich polymorphism. By employing ab initio methods, we reveal a thermodynamically stable borophene polymorph without vacancies which is a semiconductor unlike the other known boron sheets, in the form of an asymmetric centered-washboard structure. Our results indicate that asymmetric distortion is induced due to Peierls instability which transforms a symmetric metallic system into a semiconductor. We also show that applying uniaxial or biaxial strain gradually lowers the obtained band gap and the symmetric configuration is restored following the closure of the band gap. Furthermore, while the Poisson's ratio is calculated to be high and positive in the semiconducting regime, it switches to negative once the metallicity is retrieved. The realization of semiconducting borophene polymorphs without defects and tunability of its electronic and mechanical response can extend the usage of boron sheets in a variety of nanoelectronic applications

DS 35.5 Thu 10:30 CHE 89

First-principles study of hydrogenation on bilayer GaN — •Anh Khoa Augustin Lu[1], Tetsuya Morishita[1,2], Tomoe Yayama[3], and Takeshi Nakanishi[1,2] — [1]MathAM-OIL, AIST, Sendai, Japan — [2]CD-FMat, AIST, Tsukuba, Japan — [3]Department of Applied Physics, Kogakuin University, Tokyo, Japan

In the last decade, a large number of two-dimensional materials has been discovered. In recent years, two-dimensional III-V materials have arisen with the experimental demonstration of two-dimensional GaN. Here, we focus on the case of bilayer GaN. While the atomic structure of pristine bilayer GaN is relatively well understood, the impact that hydrogenation remains unclear since unlike transition metal dichalcogenides, pristine GaN has dangling bonds. In that respect, the present work focuses on the atomic structure, stability and electronic properties of bilayer GaN passivated by hydrogen atoms, with a large range of hydrogen coverage. First-principles calculations based on the density functional theory were performed to identify the structures with the lowest energy. While previous studies have focused on structures oriented along the c-plane, our results reveal that depending on the hydrogen concentration, the plane orientation of the most stable structure (c-, m-, or a-plane) is different. In particular, at high hydrogen concentration, structures oriented along the m- and a-planes have the lowest energy. Their stability is confirmed by first-principles molecular dynamics simulations performed at finite (room) temperature. By modulating the hydrogen concentration, one can therefore tailor the atomic structure and properties of bilayer GaN.