O 38: Poster 2D Materials: Stacking and Heterostructures (joint session O/HL)

Time: Tuesday 13:30–15:30 Location: P3

O 38.1 Tue 13:30 P3

Stability and electronic properties of double-layer o-B2N2 in different stacking modes — •Na Li and Claudia Draxl — Department Physics and CSMB, Humboldt-Universit at zu Berlin, D-12489 Berlin, Germany

Two-dimensional orthorhombic boron nitride (o-B2N2) has recently attracted significant attention due to its direct band gap of approximately 1.7eV and excellent visible-light absorption properties. In its layered conformations, the stacking order plays a crucial role in determining the material's stability as well as its electronic and optical properties. In this study, we employ the all-electron full potential code exciting to perform first-principles calculations of four high-symmetry bilayer stacking sequences of o-B2N2, regarding their relative stability and their electronic properties. Our calculations reveal that the AB' stacking sequence has the lowest energy and an optimized interlayer distance of 3.52 Å. The bandgaps of the AA and AA' stacking sequences are reduced relative to the monolayer, where AA' exhibits even semi-metallic behavior. In contrast, the AB and AB' stacking sequences show slightly increased direct bandgaps.

O 38.2 Tue 13:30 P3

In-depth analysis of stratified MoS2 and WS2 2D heterostructures — •Sebastian Klenk, Nikolas Dominik, Cormac Ó Coileáin, Tanja Stimpel-Lindner, and Georg S. Duesberg — University of the Bundeswehr Munich, Institute of Physics, Germany

Starting with graphene roughly two decades ago, two-dimensional (2D) materials have garnered great interest in the scientific community due to their exceptional electrical, mechanical and optical properties. The broad palette of different 2D materials has allowed for the possibility to change and finetune these parameters to one's own liking by combining several 2D materials in one film. Here, we present the metal-organic chemical vapour deposition (MOCVD) synthesis and analysis of MoS2/WS2 heterostructures. We show the ordering of a high-quality 7-layer combination structure of less than 10 nm. The layered nature is confirmed and discussed using XPS, EDX, ToF-SIMS, TEM, AFM and Raman spectroscopy.

O 38.3 Tue 13:30 P3

A Two-dimensional Heterostructure Fabrication System in Ultra-high Vacuum — •Daiyu Geng, Jiabao Yang, Natalie Lehmann, and Niels Schröter — Max Planck Institute of Microstructure Physics, Weinberg 2, Halle (Saale), Germany

We develop an ultra-high vacuum system for the fabrication of two-dimensional heterostructures. The clean transfer and stacking of two dimensional material flakes are realized using a polymer-free method based on SiNx cantilevers coated with Au film (Nature Electronics, 2023, 6(12): 981-990). The system also incorporates multiple surface preparation and characterization techniques like MBE, Plasma sputtering and electron diffraction. All these methods enable us to prepare heterostructures with atomically clean interface, which is important for the spectroscopic investigation of the rich physics effects in two-dimensional heterosystems.

O 38.4 Tue 13:30 P3

Exploring MXenes as Electrodes for Al-ion Batteries: An Ab-initio Study on the Impact of Stacking Configurations and Termination Types — •Amal Raj Veluthedath Nair and Nuala M Caffrey — School of Physics, University College Dublin, Dublin 4, Ireland

MXenes, with their tunable surface chemistry, thin 2D structures, large interlayer spacing, and good conductivity, are promising candidates for battery electrodes. The stacking configuration of MXene layers, determined by their chemistry and surface terminations, influences their electrochemical performance.

This study explores Ti_3C_2 and V_2C MXenes as electrodes for Na, Mg, and Al-ion batteries using density functional theory. We examine four stacking configurations and two coordination sites for intercalated ions. Results reveal that stacking configuration and surface terminations significantly influence change in interlayer distance, with O-terminated octahedral stacking showing the least change in spacing for all intercalants. The smallest interlayer distance change occurs for Al intercalation in V_2C, with a Δd of 0.1 Å, matching experimental findings (Vahidmohammadi et al., 2017). Ion migration studies indicate that prismatic stacking promotes faster ion migration compared to octahedral stacking. O-terminated MXenes significantly enhance the theoretical specific capacity for Al intercalation, reaching a maximum value of 283.48(277.63)mAh/g for $Ti_3C_2O_2(V_2CO_2)$. In contrast, F-terminated MXenes show much lower capacities.

O 38.5 Tue 13:30 P3

Triplet pairing enabled proximity superconductivity in monolayer WTe_2 — •A. Bäder[1,2], T. Wichmann[1,3], J. Martinez-Castro[1,4], P. Rüssmann[5,6], K. Jin[1,4], T. Samuely[7], Z. Lyu[1,3], J. Yan[8], O. Onufriienko[7], P. Szabó[7], F. S. Tautz[1,3], M. Ternes[1,4], S. Lounis[5,9], and F. Lüpke[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich — [2]II. Physikalisches Institut, Universität zu Köln — [3]Institut für Experimentalphysik IV A, RWTH Aachen — [4]Institut für Experimentalphysik II B, RWTH Aachen — [5]Peter Grünberg Institut (PGI-1), Forschungszentrum Jülich — [6]Julius-Maximilians-Universität Würzburg, Fakultät für Physik und Astronomie — [7]Centre of Low Temperature Physics, Faculty of Science, Pavol Jozef Šafárik University & Institute of Experimental Physics, Slovak Academy of Sciences — [8]Materials Science and Technology Division, Oak Ridge National Laboratory, USA — [9]Fakultät für Physik, Universität zu Duisburg-Essen

We use low-temperature scanning tunneling microscopy to investigate proximity-induced triplet pairing and its role in enabling superconductivity in a monolayer $WTe_2/NbSe_2$ van der Waals heterostructure. Employing the Kohn-Sham Bogoliubov-de Gennes formalism, we find that conventional s-wave pairing fails to induce superconductivity in the WTe_2, in contrast to triplet pairing. Applying an external magnetic field, we examine Abrikosov flux vortices within the heterostructure and exploit them to probe local superconducting properties. Our findings highlight a platform for studying triplet pairing-induced superconductivity with potential topological characteristics.