CPP 6: 2D Materials (joint session CPP/O)

Time: Monday 11:30–12:15 Location: ZEU 255

CPP 6.1 Mon 11:30 ZEU 255

Voltage-dependent quantitative analysis of electron-dose-limited resolution for imaging two-dimensional covalent organic framework — •Baokun Liang[1], Haoyuan Qi[1,2], Hafees Sahabudeen[2], Xinliang Feng[2], and Ute Kaiser[1] — [1]Central facility for Electron Microscopy, Group of Electron Microscopy of Materials Science, University of Ulm, 89081 Ulm, Germany — [2]Department of Chemistry and Food Chemistry & Center of Advancing Electronics Dresden, Dresden University of Technology, 01062 Dresden, Germany

Two-dimensional covalent organic framework (2D COF) are promising candidates for organic electronics and next-generation energy storage. However, due to electron irradiation damage, high resolution (HR) TEM imaging of 2D COFs remains challenging, posing a substantial limitation on the structural elucidation of these organic 2D materials. Therefore, it is necessary to unravel the correlation between total electron dose and achievable specimen resolution for specific specimens. To investigate the relationship between total electron dose and achievable specimen resolution, we performed a dose-series analysis with 2D COF in electron diffraction mode under different acceleration voltages (300, 200, 120, 80 kV). With accumulating electron dose, the higher-order reflections gradually vanish, representing the degradation of specimen resolution. For quantitative analysis, the intensity of reflections within a specific resolution band was analyzed. Our method offers a quick and straightforward determination of dose-related specimen resolution under different voltages. These results lay the foundation for the HRTEM imaging of beam sensitive 2D COFs.

CPP 6.2 Mon 11:45 ZEU 255

Solvent interactions with two-dimensional materials: A computational investigation of the dispersion of graphene monolayers in commonly-used solvents. — •Urvesh Patil and Nuala Caffrey — School of Physics & CRANN, Trinity College, Dublin 2

Maintaining stable dispersions of two-dimensional (2D) materials is a prerequisite for several applications. The stability of dispersion, i.e., the ability of a solvent to maintain an adequate concentration of suspended flakes over time, depends strongly on the interaction between the 2D material and the chosen solvent. In order to identify the optimal solvent for a particular 2D material it is imperative to determine this interaction on the atomic scale. Here, we use density functional theory (DFT) combined with solvent models and molecular dynamics (MD) to study the interaction of graphene and MoS2 with solvent molecules such as NMP, cyclopentanone and toluene. Using DFT, we show that isolated solvent molecules interact via a van der Waals (vdW) interaction with pristine monolayers, with negligible charge transferred between them. MD calculations show that distinct solvation shells form around the 2D layer; the first solvation shell is formed as a result of vdW interaction irrespective of the polarity of solvent. This then interacts with rest of the solvent via a combination of both electrostatic and vdW forces. We show that the formation of this solvation shell is always favourable, and determine the relationship between the free energy of interaction and the experimental concentration of graphene in solution. Finally, we suggest a simple rule for mixing solvents that can be used to improve the 2D layer concentration in solution.

CPP 6.3 Mon 12:00 ZEU 255

Relation between topology and electronic structure of 2D polymers — •Maximilian A. Springer[1,2], Tsai-Jung Liu[2], Agnieszka Kuc[1], and Thomas Heine[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Resource Ecology, Research Site Leipzig, Permoserstrasse 15, 04318 Leipzig, Germany — [2]TU Dresden, Faculty of Chemistry and Food Chemistry, Bergstrasse 66c, 01062 Dresden, Germany

New 2D materials open access to a whole new world of compounds and properties. Graphene monolayer is such a material, since it has special electron transport features due to its honeycomb topology. Apart from the honeycomb net, there are many more 2D topologies which promise a manifold of new properties, e.g. the kagomé or the Lieb lattice. As recently shown in the case of the kagomé net, 2D polymers (covalent organic frameworks) can be designed in a way that their geometric and electronic structure match the desired topology [Y. Jing, T. Heine, J. Am. Chem. Soc. 2019, 141, 2, 743-747]. We investigate electronic properties including topological signatures of different 2D nets using a tight-binding approach. Based on these findings, we want to propose new 2D polymers with the desired structures and new properties using density-functional theory.