

CPP 54: 2D Materials VIII

Time: Thursday 16:30–17:45

Location: MER 02

CPP 54.1 Thu 16:30 MER 02

Structure elucidation of 2D covalent organic frameworks — ●MARYKE KOUYATE^{1,3}, KONRAD MERKEL¹, DOMINIK PASTOETTER², ALBRECHT LUDWIG WAENTIG², XINLIANG FENG², and FRANK ORTMANN¹ — ¹Technical University of Munich, Munich, Germany — ²TU Dresden, Dresden, Germany — ³Fritz Haber Institute of the Max Planck Society, Berlin, Germany

We determine the structure of novel 2D framework materials (known as 2D polymers or 2D COFs) that are based on Diquinoxalino[2,3-a:2',3'-c]phenazine (HATNA) vertex units and different linkers (naphthalene vs. pyrene). We simulate the unit cell parameters and stacking patterns with density functional theory. The studied COFs were synthesized and experimentally characterized by our collaborators. Our theoretical studies include extensive xyz scans to find the most energetically favorable stacking geometry. With the results of the xyz scans and the appropriate selection of the unit cell, good agreement is obtained with the experimental PXRD patterns, and individual XRD peaks can be assigned to specific in-plane or out-of-plane directions. Moreover, the simulated structures show a clear difference in the packing of the two COFs which are caused by differences in their linker units. This observation is also consistent with the differences in the experimental PXRD patterns. As a result, we can shed light on the actual cell parameters and stacking behavior.

CPP 54.2 Thu 16:45 MER 02

How to calculate electron-hole interaction efficiently in large covalent organic frameworks? — ●KONRAD MERKEL and FRANK ORTMANN — TU München, School of Natural Sciences

Solving the Bethe-Salpether equation for crystalline materials with many atoms per unit cell, such as covalent organic frameworks, is computationally very expensive and often not feasible. Established tools are usually not suitable for this class of materials because they have enormous memory requirements due to their large basis sets. An elegant solution is to use material-specific, tailored basis sets that allow a complete description with only a handful of basis functions and therefore require only a fraction of the computational resources. In our talk, we present a technique using Wannier functions as a suitable basis and computing Coulomb matrix elements in this basis. The fully parameterized exciton Hamiltonian is then solved using a linear scaling approach that allows efficient computation of spectral quantities such as the exciton DOS for materials with hundreds of atoms per unit cell.

CPP 54.3 Thu 17:00 MER 02

New Paradigm for Gas Sensing by Two-Dimensional Materials — ●UDO SCHWINGENSCHLÖGL, VASUDEO BABAR, and SITANSH SHARMA — King Abdullah University of Science and Technology (KAUST), Physical Science and Engineering Division (PSE), Thuwal 23955-6900, Saudi Arabia

The adsorption behavior and electronic transport properties of CO and NH₃ molecules on para-C₃Si and meta-C₃Si monolayers are studied using first-principles calculations and the non-equilibrium Green's

function method. The adsorption sites are determined along with their adsorption energies. It turns out that CO and NH₃ molecules physisorb on both monolayers. The current-voltage characteristics show that the para-C₃Si monolayer can be used to sense CO and NH₃ gases with high sensitivity. In contrast to other two-dimensional materials, the sensing mechanism is not based on charge transfer but on the presence of Dirac states and their susceptibility to symmetry-breaking structural distortions. Journal Reference: J. Phys. Chem. C 123, 13104 (2019)

CPP 54.4 Thu 17:15 MER 02

Tunable gas permeation properties through sub-nanometer porous molecular thin carbon nanomembranes — ●VLADISLAV STROGANOV¹, DANIEL HÜGER¹, TABATA NOETHEL¹, CHRISTOF NEUMANN¹, MONIKA KRUK², PIOTR CYGANIK², and ANDREY TURCHANIN¹ — ¹Friedrich Schiller University Jena, Jena, Germany — ²Jagiellonian University, Kraków, Poland

Molecular thin carbon nanomembranes (CNMs) are 1 nm thick nanosheets with sub-nanometer porosity combined with high mechanical and chemical stability. These properties make them promising for the next generation of filtration and gas separation technologies. Here we investigated influence of the structure of molecular precursors on the gas permeation properties of a series of CNMs. The CNMs were synthesized from self-assembled monolayers of biphenyl substituted carboxylic acids on silver substrate C₆H₅-C₆H₄-(CH₂)_n-COO|Ag (n = 2 - 6) via the electron-irradiation induced cross-linking. We study for this homologous sequence of CNMs the permeation of He, D₂ and D₂O vapors as a function of temperature. We demonstrate that even a smallest variation of the number of -CH₂- units leads to a significant change in the permeation which enables the molecular design of these nanomembranes for nanofiltration.

CPP 54.5 Thu 17:30 MER 02

Vapor Adsorption on CNMs studied with Infrared Spectroscopy — ●JAKOB KREIE, PETR DEMENTYEV, NEITA KHAYYA, and ARMIN GÖLZHÄUSER — Physics of Supramolecular Systems and Surfaces, Bielefeld University, Germany

Carbon nanomembranes (CNM) are made by electron induced cross-linking of aromatic self-assembled monolayers. Previous studies show that CNM enable rapid transport of water vapor. This may be related to a strong adsorption of water molecules on the CNM surface. A spectroscopic setup for infrared measurements of vapor adsorption on CNMs is designed to investigate the adsorption on the surface under realistic conditions. For this purpose, a reaction chamber in a polarization-modulation infrared reflection absorption spectroscopy (PM IRAS) is connected to a vacuum system in order to be able to control the vapor environment.

First measurements are performed with a terphenyl-4-thiol carbon nanomembrane (TPT-CNM). The results show that even low vapor pressures of heavy water are sufficient to achieve strong adsorption on the surface of the TPT-CNM, which indicates a large influence of the surface effects on water transport through the membrane.