CPP 11: 2D Materials 3 (joint session CPP/DS)

Time: Monday 17:15–17:45 Location: H38

CPP 11.1 Mon 17:15 H38

On the electronic pi-system of 2D covalent organic frameworks — •Konrad Merkel, Johannes Greiner, and Frank Ortmann — TU München

We investigate a family of 2D hexagonal covalent organic frameworks (COFs) with different linker monomers regarding their electronic structure and pi-conjugation. Molecular orbitals can be obtained from maximally localized Wannier functions and turn out to be sigma- and pi-like orbitals forming distinct sigma- and pi-bands, respectively. The Wannier description enables a detailed analysis of the topology, effective coupling and delocalization of the entire pi-system. We identify conjugated states that are delocalized across multiple building blocks of the COF and show their robustness against perturbations like out-of-plane rotations of molecular fragments and different strength of Anderson disorder. Furthermore, we apply the nucleus-independent chemical shift (NICS), which is an established measure of aromaticity. All results are compared for different types of linker units with different degrees of pi-conjugation.

CPP 11.2 Mon 17:30 H38

Permeation of gases through molecularly thin carbon nanomembranes — •Vladislav Stroganov[1], Daniel Hüger[1], Tabata Nöthel[1], Christof Neumann[1], Uwe Hübner[2], Michael Steinert[1], Monika Kruk[3], Piotr Cyganik[3], and Andrey Turchanin[1] — [1]Friedrich-Schiller University Jena, Jena, Germany — [2]Leibniz Institute of Photonic Technology, Jena, Germany — [3]Jagiellonian University, Kraków, Poland

Atomically thin carbon nanomembranes (CNMs) are promising candidates for next generation filtration and gas separation technologies. However, the gas permeation mechanism through CNMs is not fully understood yet. To improve this knowledge, we investigated permeation of helium, deuterium, water vapor and other gases through a series of CNMs under different conditions. The CNMs were synthesized from biphenyl substituted carboxylic acids on silver substrate $C_6H_5-C_6H_4-(CH_2)_n-COO|Ag$, with different lengths of aliphatic linker n = 2 - 6. A CNM based on terphenyl thiol (TPT) was used as a well-known reference system. We demonstrated that even the smallest variation in the structure of the molecular precursor lead to significant change of the permeation properties.