CPP 44: 2D Materials

Time: Friday 11:30–12:30 Location: H34

CPP 44.1 Fri 11:30 H34

Sensors based on graphene field-effect transistors functionalized with molecularly imprinted polymers — •David Kaiser[1], Hamid Rasouli[1], Michael Ringleb[2,3], Ludwig Büttner[2], Martin Hager[2,4], Guobin Jia[5], Jonathan Plentz[5], Christian Beringer[4], Patrick Bräutigam[4], Uwe Hübner[5], Patrick Endres[2], Christof Neumann[1], Steffi Stumpf[2,3], Benjamin Dietzek-Ivanšić[1,4,5], Ulrich S. Schubert[2,3,4] und Andrey Turchanin[1,3,4] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena — [2]Laboratory of Organic and Macromolecular Chemistry, Friedrich Schiller University Jena — [3]Jena Center for Soft Matter, Friedrich Schiller University Jena — [4]Center for Energy and Environmental Chemistry Jena, Friedrich Schiller University Jena — [5]Leibniz Institute of Photonic Technology (Leibniz IPHT)

Monitoring of micropollutants has become a regulatory requirement due to their environmental and health impacts. However, their on-site detection remains challenging, as current methods require transporting samples to centralized laboratories. Here, we present a method for the direct identification of the pharmaceutical carbamazepine (CBZ) utilizing solution-gated graphene field-effect transistors (SG-GFETs) that is appropriate for on-site use. We integrate molecularly imprinted nanoparticles (MIPs) with a diameter of 20 nm onto graphene via their self-assembly, creating highly stable films that specifically bind CBZ, and demonstrate a detection sensitivity reaching as low as 1 pM in buffer solutions and 10 pM in samples of environmental water.

CPP 44.2 Fri 11:45 H34

Efficient DFT Band Gap Correction for 2D-Covalent Organic Frameworks Towards Hybrid Functional Level — •Laura Fuchs and Frank Ortmann — Technische Universität München, TUM School of Natural Sciences

Density functional theory (DFT) is the workhorse computational tool for predicting the structure and physical properties of inorganic and organic molecules as well as semiconductors. Unfortunately, the optical and fundamental band gaps are not well described by semi-local DFT approaches. In particular, common DFT methods like the local density approximation (LDA) and the generalized gradient approximation (GGA) severely underestimate the fundamental band gaps, which is commonly referred to as the "band gap problem". However, the correct band gap is of utmost importance for evaluating the suitability of materials such as organic semiconductors for applications like photocatalysis or green energy harvesting. Besides highly expensive many-body perturbation theory, hybrid functionals can address the band gap problem. However, these functionals still involve high computational costs and, for large two-dimensional covalent organic frameworks (2D-COFs), these efforts are not always feasible. Here, we study the relation between semi-local PBE and hybrid HSE06 functionals and present a simple and computationally cheap scheme to extrapolate the PBE band gaps in 2D-COFs to a more precise band gap at HSE06 level.

CPP 44.3 Fri 12:00 H34

Towards the Computational Design of Molecular Olfactory Receptors for Digital Odor Detection — •Li Chen[1], Leonardo Medrano Sandonas[1], Arezoo Dianat[1], Nina Tverdokhleb[1], Rafael Gutierrez[1], Alexander Croy[2], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center for Biomaterials, TUD Dresden University of Technology, 01062 Dresden, Germany — [2]Institute of Physical Chemistry, Friedrich Schiller University Jena

We present the MORE-Q dataset using quantum-mechanical (QM) simulations for dimer systems composed of body odor volatilome (BOV) and olfactory receptors. The dataset contains abundant QM properties of diverse BOV-receptor systems, both in the gas phase and when deposited on a graphene surface. After analyzing the property space spanned by MORE-Q, we observed flexibility when searching for a dimer configuration with a desired set of electronic binding features. To gain insights into the complex interplay between these sensing properties, an ensemble learning method (XGBoost) was constructed for the fast evaluation of BOV adsorption behavior using only the dimer configurations properties. The results show a significant increase in model performance by adding multiple conformers to the training procedure, and SHAP analysis identifies the most relevant descriptors for predicting the binding features. Our work provides valuable insights into the the sensing mechanism of BOV molecules and paves the way for the computational design of receptors with targeted sensitivity and selectivity.

CPP 44.4 Fri 12:15 H34

Effective EMI shielding solutions: the role of 2D materials and their performance across frequency ranges — •Reyhaneh Bahramian[1,2] and Mohammad Nezafati[2] — [1]Department of Cognitive Sciences, Faculty of Psychology and Education, University of Tehran, Tehran, Iran — [2]Condensed Matter National Laboratory, Institute for Research in Fundamental Sciences, Tehran 19395-5531, Iran

The rise in electronic device usage has led to increased electromagnetic interference (EMI), creating a pressing need for effective shielding materials that are flexible, lightweight, cost-efficient, and high-performing. Two-dimensional (2D) materials are emerging as strong candidates for next-generation EMI shielding solutions. This review examines the origins of electromagnetic responses and shielding mechanisms, focusing on photon-matter interactions, and evaluates the instruments and standards for measuring shielding effectiveness.

Recent advancements in 2D materials for EMI shielding are analyzed, comparing their performance across different frequency ranges with other composite materials. Although 2D material-based composites show significant promise, challenges remain in expanding their applications, particularly in the sub-gigahertz range.