# CPP 7: Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods I

Time: Monday 11:30–12:45 Location: ZEU/0255

CPP 7.1 Mon 11:30 ZEU/0255

**Exploration of quantum-mechanical space towards olfactorial receptor and body odor volatilomes interaction** — •Li Chen[1], Leonardo Medrano Sandonas[1], Shirong Huang[1], and Gianaurelio Cuniberti[1,2] — [1]Institute for Materials Science and Max Bergmann Center for Biomaterials, TUD Dresden University of Technology, 01062 Dresden, Germany — [2]Dresden Center for Computational Materials Science (DCMS), TUD Dresden University of Technology, 010628 Dresden, Germany

We present the MORE-QX dataset generated from quantum-mechanical (QM) simulations of atomistic systems spanning diverse design stages for gas sensing. The dataset contains 23,838 and 10,441 BOV*receptor dimer systems in the gas phase and on graphene surfaces, respectively, to obtain sensing-related binding features. By analyzing the property space spanned by MORE-QX, we observe substantial flexibility in identifying interaction configurations with desired electronic binding characteristics, owing to the weak correlations among the properties. To gain insights into the complex interplay between these sensing properties, we construct tree-based machine-learning models for fast evaluation of binding features using only QM molecular properties, and combine them with an explainability framework to identify the key design factors of BOV*receptor systems that govern sensing performance. Our work provides valuable insights into the sensing mechanism and design principles of olfactorial receptors for BOV sensing.

CPP 7.2 Mon 11:45 ZEU/0255

**Non-local diffusion model as a description for non-Gaussian diffusion in scattering experiments** — •Harish Srinivasan[1,2], Veerendra Kumar Sharma[2], and Subhankur Mitra[2] — [1]Institute of Applied Physics, University of Tübingen, Tübingen, Germany — [2]Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai, India

We introduce a non-local diffusion (NLD) model that provides a unified theoretical framework for describing non-Gaussian diffusive dynamics in fluids. The NLD formulation generalizes conventional diffusion by incorporating a jump kernel, enabling analytical characterization of van-Hove self-correlation functions with exponential tails. This framework naturally connects two major classes of anomalous transport observed in scattering experiments: non-Gaussian fractional Brownian motion (nGfBm) in sub-diffusive glass-formers, and Fickian yet non-Gaussian diffusion (FnGD) in cage-jump dominated liquids. In the nGfBm regime, the NLD description captures the crossover from non-Gaussian to Gaussian sub-diffusion seen in molecular and polymeric glass-formers [1]. In the FnGD regime, the NLD model predicts the exponentially fast approach to Fickianity and the much slower algebraic restoration of Gaussianity [2]. Comparison with incoherent quasielastic neutron scattering data across multiple systems demonstrates the universal applicability of the NLD model and establishes non-local diffusion as the common physical origin of non-Gaussian signatures in molecular fluids. [1] H. Srinivasan et. al., Phys. Rev. Lett. 132, 058202 (2024) [2] H. Srinivasan et. al., arXiv:2504.15020 (2025)

CPP 7.3 Mon 12:00 ZEU/0255

**Optimizing EquiDTB potentials for large-scale molecular simulations** — •Zekiye Erarslan, Gianaurelio Cuniberti, and Leonardo Medrano Sandonas — Chair of Materials Science and Nanotechnology, TUD Dresden University of Technology, 01062 Dresden, Germany

Density Functional Tight-Binding (DFTB) is a semi-empirical method that enables efficient large-scale simulations at moderate computational cost compared to first-principles quantum-mechanical methods. However, its generalizability is limited by the use of parameterized pairwise repulsive potentials. The recently developed EquiDTB framework [chemRxiv, 10.26434/chemrxiv-2025-z3mhh] has shown that replacing this repulsive term with a many-body ΔTB potential—trained using equivariant neural networks—significantly improves both the accuracy and transferability of the DFTB method. As a result, EquiDTB achieves hybrid DFT-PBE0 level accuracy across diverse electronic, structural, and vibrational properties of large molecules and molecular dimers containing C, N, O, and H atoms. In this work, we extend the EquiDTB framework by training a more general ΔTB potential on the chemical space covered by the newly generated QCML dataset. This expansion broadens EquiDTB beyond its original four-element scope and enables accurate simulations of neutral molecular systems containing C, N, O, H, P, S, Na, and Cl. We validate the performance of the optimized EquiDTB model through extensive calculations on large molecular dimers, RNA systems, and organic periodic materials.

CPP 7.4 Mon 12:15 ZEU/0255

**MolecuTas: an ML platform for refining quantum properties and bioactivity of complex molecules** — •Álvaro Vallejo Bay[1], Jannis Krüger[2], Thomas Hellweg[2], Gerardo Prieto[1], and Vicente Domínguez Arca[2,3] — [1]Applied Physics, University of Santiago de Compostela, Spain — [2]Physical and Biophysical Chemistry, Bielefeld University, Germany — [3]Biosystems and Bioprocesses Engineering, IIM-CSIC, Spain

This work introduces MolecuTas, a neural architecture designed for the ultrafast prediction of atomistic and molecular properties with accuracy approaching density functional theory, yet at negligible computational cost. The project tackles core challenges in computational chemistry, particularly the size dependence of predictive models and the loss of structural detail in conventional representations. To overcome these limitations, we develop a custom data extraction and molecular fragmentation pipeline based on large quantum datasets, ensuring the preservation of essential information such as connectivity, symmetries, chemical environments, and electronic features.

Building on this foundation, we propose a family of advanced Graph Neural Networks that explicitly integrate physicochemical principles and disentangle local from global information, enabling robust generalization across diverse molecular systems. Ultimately, MolecuTas aims to provide a reliable tool for molecular dynamics, enabling precise and fast prediction of partial charges and other key descriptors required for accurate simulations and next-generation chemical design.

CPP 7.5 Mon 12:30 ZEU/0255

**Property-guided diffusion modeling for efficient exploration of chemical spaces** — •Leonardo Medrano Sandonas[1], Michael Hanna[1], Julian Cremer[2], and Gianaurelio Cuniberti[1] — [1]TUD Dresden University of Technology, Germany. — [2]Pfizer Worldwide R&D, Germany.

The rational in silico design of chemical compounds requires a deep understanding of both structure-property and property-property relationships across chemical compound space, as well as efficient methodologies for defining inverse property-to-structure mappings. In this presentation, I will discuss our recent efforts to leverage the "freedom of design" concept [Chem. Sci. 14, 10702 (2023)] in the chemical space of drug-like molecules to develop an efficient generative AI framework capable of designing molecular compounds with targeted quantum-mechanical (QM) properties. To this end, we have implemented a property-guided active learning approach that optimizes the performance of equivariant diffusion models within each property space. Generated molecules and their associated QM properties are validated through exhaustive DFT calculations at the PBE0+MBD level using the FHI-aims code. Our findings reveal a consistent improvement in property accuracy when guiding the diffusion model to explore less populated regions of the target property space. This performance is further enhanced by incorporating molecular building blocks into the initial training set. We expect our work to advance the development of sustainable generative AI frameworks for identifying molecules tailored to specific chemical processes.