

## CPP 14: 2D Materials

Time: Monday 16:15–17:45

Location: H 0111

CPP 14.1 Mon 16:15 H 0111

**Molecular dynamics dimulation: exploring human odorant adsorption on functionalized 2D carbon surfaces. Workflow.**

— •NINA TVERDOKHLEB<sup>1</sup>, LI CHEN<sup>1</sup>, AREZOO DIANAT<sup>1</sup>, RAFAEL GUTIERREZ<sup>1</sup>, ALEXANDER CROY<sup>2</sup>, and GIANAURELIO CUNIBERTI<sup>1</sup> — <sup>1</sup>Institute for Materials Science, Dresden University of Technology, Dresden 01062, Germany — <sup>2</sup>Institute of Physical Chemistry, Friedrich Schiller University Jena, 07737 Jena, Germany

Our group explores the sensory properties of graphene and nanotubes functionalized with mucin-based smell receptors specifically designed to detect human odorant molecules. This involves a molecular dynamics simulation using the NAMD software to analyze interactions between pools of receptors and odorants in the gaseous phase. The adsorption energy of odorants on functionalized graphene is assessed using The Adaptive Biasing Force (ABF) Method [1], revealing correlations with structural characteristics. Moreover, we ascertain the receptor recovery time through the application of the Arrhenius law, and extract temporal associations from molecular dynamic trajectories. This approach holds the promise of fostering a more profound understanding of the sensory mechanisms, contributing to the development of electronic olfaction for enhanced disease detection.

[1] Eric Darve, David Rodríguez-Gómez, and Andrew Pohorille. Adaptive biasing force method for scalar and vector free energy calculations. *J. Chem. Phys.*, 128(14):144120, 2008.

CPP 14.2 Mon 16:30 H 0111

**Radioactive Tracer Diffusion through TPT-CNMs** — •NEITA KHAYYA, ANDRÉ BEYER, and ARMIN GÖLZHÄUSER — Faculty of Physics, Bielefeld University, 33615 Bielefeld, Germany

In recent years, Carbon Nanomembranes (CNMs) have emerged as an innovative class of thin 2D materials known for their exceptional combination of high selectivity and permeation properties, with a particular emphasis on p-[1,1',4',1'']-terphenyl-4-thiol (TPT)-CNM. Despite significant progress in comprehending the characteristic features of CNMs, there remains a need for further clarification of their fundamental properties, which can be addressed through complementary methods. Here, we report the permeation measurements derived from concentration-gradient-driven transport of radioactive tracer molecules, specifically [3H] H<sub>2</sub>O, [14C] NaHCO<sub>3</sub>, and [32P] H<sub>3</sub>PO<sub>4</sub>, through TPT-CNMs. Our investigation explores into the impact of the pH value on the diffusion process. Considering concentration polarization and outgassing effects by a mathematical model, our results align with previously obtained radioactive diffusion data for a neutral pH value of 7. Interestingly, despite the electrostatic barrier associated with TPT-CNM, our observations indicate enhanced permeation of anions in the basic range of pH. This emphasizes the nuanced behavior of TPT-CNMs under varying pH conditions, shedding light on their unique permeation characteristics.

CPP 14.3 Mon 16:45 H 0111

**Theoretical Studies on the Formation of Polymeric Nitrogen-containing 2D-Networks of Tricyanobenzene Derivatives on Coinage Metal Surfaces** — •ALIX KACZMAREK<sup>1,2</sup>, JÖRG SUNDERMEYER<sup>3</sup>, and DOREEN MOLLENHAUER<sup>1,2</sup> — <sup>1</sup>Institute of Physical Chemistry, Justus-Liebig University Giessen, Germany — <sup>2</sup>Center for Materials Research (LaMa), Justus-Liebig University Giessen, Germany — <sup>3</sup>Chemistry Department, Philipps-University Marburg, Germany

The field of metal surface chemistry, and on-surface reactions in particular, has attracted considerable attention in recent years. The development of fundamental strategies for on-surface synthesis through the investigation of the underlying reaction mechanisms will provide a toolbox for applications in various fields such as photonics, photo- and electrocatalysis, or solar energy conversion. E.g. 2D graphene-like nitrogen-containing 'azagraphene' networks are a promising class of systems for use in nanoscale electronic devices. Here, we present the investigation of the trimerisation mechanisms of planar 1,3,5-tricyanobenzene (TCB) and 2,4,6-tricyano-1,3,5-triazine (TCT) on (111) coinage metal surfaces copper, silver, and gold, using density functional theory with dispersion correction. Our findings may provide guidance for the experimental synthesis of nitrogen-containing graphene networks and aid in the selection of suitable precursor-

surface-systems.

L. Alix Kaczmarek, Michael Gottfried, Jörg Sundermeyer, Doreen Mollenhauer. Manuscript in preparation.

CPP 14.4 Mon 17:00 H 0111

**Atomistic simulation of a novel non-covalent functionalized graphene-based sensor material for body odor volatiles detection** — •LI CHEN<sup>1</sup>, NINA TVERDOKHLEB<sup>1</sup>, AREZOO DIANAT<sup>1</sup>, RAFAEL GUTIERREZ<sup>1</sup>, ALEXANDER CROY<sup>2</sup>, and GIANAURELIO CUNIBERTI<sup>1</sup> — <sup>1</sup>Institute for Materials Science, Dresden University of Technology, Dresden 01062, Germany — <sup>2</sup>Institute of Physical Chemistry, Friedrich Schiller University Jena, 07737, Jena, Germany

Detecting the body odor volatiles (BOVs) represents a crucial step in comprehending its implications for human social interactions and healthcare. This work explores a novel mucin-based receptor functionalized graphene-based sensor material for BOVs detection through atomistic simulations. The density functional theory (DFT) investigation involves calculating the binding features of analyte-substrate interactions, including binding energy and charge transfer. These electronic properties characterize the sensing mechanisms and yield synergistically sensor signal response in the end, which could be estimated by the work function change before and after BOVs adsorption. This research enhances the fundamental understanding of the analyte-receptor interactions and potentially facilitates the selection and optimization of the receptors in pursuit of high responsiveness and excellent discrimination capabilities.

CPP 14.5 Mon 17:15 H 0111

**Defect-Healed Carbon Nanomembranes for Enhanced Salt Separation: Scalable Synthesis and Performance** — •ZHEN YAO<sup>1</sup>, PENGFEI LI<sup>1,2</sup>, KUO CHEN<sup>1,2</sup>, YANG YANG<sup>1</sup>, ANDRÉ BEYER<sup>1</sup>, QINGSHAN NIU<sup>3</sup>, and ARMIN GÖLZHÄUSER<sup>1</sup> — <sup>1</sup>Bielefeld University, 33615 Bielefeld, Germany — <sup>2</sup>China University of Petroleum (East China), Qingdao 266580, PR China — <sup>3</sup>Shenzhen University, Shenzhen 518060, PR China

Carbon nanomembranes (CNMs), featuring a high density of sub-nanometer channels, enable superior salt separation performance compared to conventional membranes. However, defect occurrence during synthesis and transfer processes impedes their technical realization on a macroscopic scale. Here, we introduce a practical and scalable interfacial polymerization method to effectively heal defects while preserving the sub-nanometer pores within CNMs. The defect-healed CNMs exhibit exceptional performance in forward osmosis (FO), achieving a water flux of 105 L m<sup>-2</sup> h<sup>-1</sup> when measured with 1M NaCl as draw solution. This water flux is ten times higher than commercially available FO membranes. Through successful implementation of the defect-healing method and support optimization, we demonstrate the scalable synthesis of fully functional, centimeter-scale CNM-based composite membranes, showing a water permeance comparable to commercial membranes and a salt rejection of ~99.8%. Our defect-healing method presents a promising pathway to overcome limitations in CNM synthesis, unlocking their potentials for practical salt separation applications.

CPP 14.6 Mon 17:30 H 0111

**Theoretical Studies of the Influence of Different XC-Functionals and Dispersion Corrections on Surface Assisted Reactions and Comparison with Theory of a Higher Level** — •KIYAN LINUS HAIKO POHL<sup>1,2</sup>, JANNIS JUNG<sup>1,2</sup>, and DOREEN MOLLENHAUER<sup>1,2</sup> — <sup>1</sup>Institute of Physical Chemistry, Justus-Liebig University Giessen, Germany — <sup>2</sup>Center for Materials Research (LaMa), Justus-Liebig University Giessen, Germany

Experimental and theoretical studies of on-surface reactions, such as the surface assisted Ullmann-coupling, have become of increasing interest in the recent years, as they provide a promising path to e. g. 2D graphene like structures. Density functional theory (DFT) is mainly used for the theoretical studies, and a variety of different exchange-correlation (XC) functional and dispersion correction combinations are available for the calculations.

We investigated combinations of 22 XC functionals and 5 dispersion corrections for the Ullmann coupling reaction of bromobenzene on the (111) coinage metal surfaces of copper, silver, and gold. We studied the influence of these combinations on different steps of the reaction.

First, the lattice parameters and the structure of the molecule were calculated and compared with experimental or benchmark values (at the CCSD(T) theoretical level). Second, the adsorption energies and

the distances of the molecules and radicals from the surface were also studied and compared to each other [1].

[1] Pohl, K. L. H., Mollenhauer, D., Manuscript in preparation.