CECAM Flagship Workshop

Virtual Materials Design: AI, Simulation, and Workflows

June 2, 2025 - June 5, 2025

Poster Overview

Please bring all posters (A0) on Monday and pin them up (pins provided)

All posters will be **displayed throughout the Workshop**, at least Monday and Tuesday.

Please present your poster in the following session:

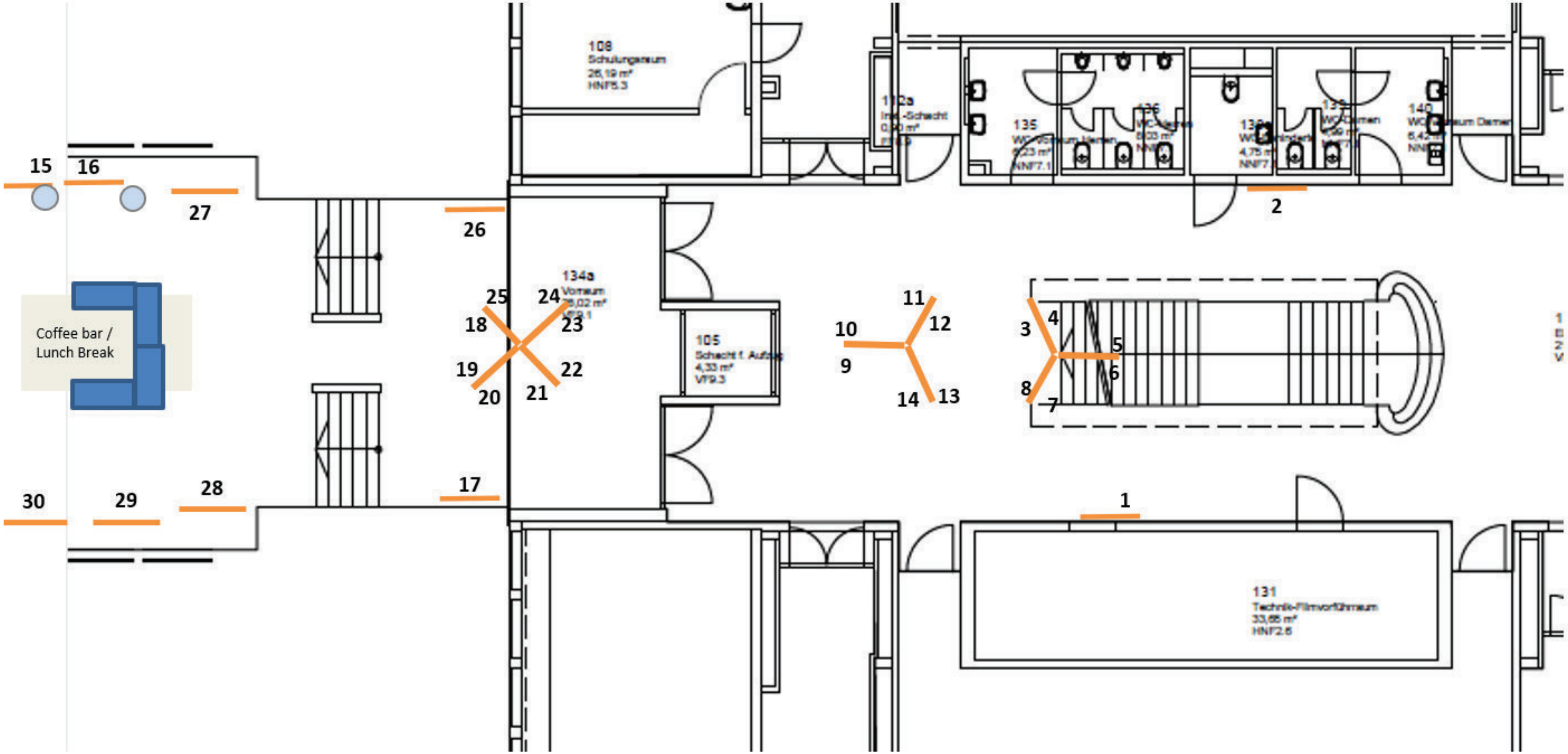
Monday 2nd June 2025 18:45 Session 1

Poster Place #	Name
1	Isaac Mackley
3	José Maria Castillo Robles
5	Amol Verma
7	Amir Kleiner
9	David Bienek
11	Laura Bianca Pasca
13	Litong Wu
15	Sebastian Will
17	Pierluigi Strazzanti
19	Mostafa Salimi
21	Sipra Mohapatra
23	Nikita Matsokin
25	Rodrigo Cortes Mejia
27	Dominique Buyens
28	Muhammed Jeneesh Kariyottukuniyil
29	Shixuan Su

Tuesday 3rd June 2025 13:00 Poster Session 2

Poster Place #	Name
2	Milan Kočí
4	Abdelrahman Elrawy
6	Alexandros Tzanakakis
8	Daniele Asnicar
10	Abdullah Bin Shahid
12	Mirko Fischer
14	Aaron Gadzekpo
16	Philipp Dullinger
18	Lobna Saeed Abdelrazik Aly
20	Salma Naimi
22	Soumya Mondal
24	Jatin Kansal
26	Mariana Kozlowska

Poster Place #	Name	Title
Monday		
1	Isaac Mackley	Effect of Nitrogen Incorporation in Amorphous HfO2
3	José Maria Castillo Robles	Probing Ultrafast Dynamics in Battery Cathodes with Automated Workflows
5	Amol Verma	AB INITIO STUDY OF POINT DEFECTS IN TUNGSTEN METAL
7	Amir Kleiner	Modeling exciton dynamics on WS2 monolayers under inhomogeneous strain from first principles
9	David Bienek	Predicting The Ionic conductivity From the Structure of Ionic Liquids with the Help of Machine Learning
11	Laura Bianca Pasca	Machine-learning-driven modelling of amorphous and polycrystalline perovskite systems
13	Litong Wu	The Zintl–Klemm Concept in the Amorphous State: A Case Study of Na–P Battery Anodes
15	Sebastian Will	Development of a Charge Propagation Workflow for Organic Semiconductors
17	Pierluigi Strazzanti	classical and machine learning force fields for carbon dioxide
19	Mostafa Salimi	Ab-Initio Investigation of the Aqueous Nafion-Platinum Interface for Enhanced PEM Fuel Cell Performance
23	Nikita Matsokin	Multi-scale Modeling of Ethylene Oligomerization on Ni-NU-1000: From DFT and GCMC/MD to Kinetic Mechanism
21	Sipra Mohapatra	Advances in CO_2 Reduction Using MOFs: A Computational Approach
25	Rodrigo Cortes Mejia	Integrating Workflows, HPC, and Domain Packages for Materials Science: a closer look at TextS
27	Dominique Buyens	Coherence locking in a parallel NMR probe defends against gradient field spillover
29	Shixuan Su	Atomic Structure of Amorphous $Ge_2Sb_2Te_5$: Machine Learning Potentials and Hybrid Reverse Monte Carlo Simulation
28	Muhammed Jeneesh Kariyottukuniyil	Enhancing the Lifetime of Triplet Excitons Through Controlled Intermolecular Interactions
Tuesday		
2	Milan Kočí	Efficient Exploration of Phase Space for Organic Molecules on Ionic Crystal Surfaces using FireCore and GPU Acceleration
4	Abdelrahman Elrawy	Deep learning assisted investigation of drug-carrier interactions using drying droplet patterns
6	Alexandros Tzanakakis	A Hierarchical Variational Autoencoder for Polymer Design using Fused Latent Representations
8	Daniele Asnicar	Linking structure and (chir)optical properties of self-assembling systems: A porphyrin-peptide conjugate as a case study
10	Abdullah Bin Shahid	High-Throughput Computational Screening of Silanes for Tire Applications: Bridging Atomistic Simulations and Macroscopic Performance
12	Mirko Fischer	Insights into modeling polymers with Machine Learning Interatomic Potentials using model systems
16	Philipp Dullinger	Machine learning for Molecular Dynamics Simulations (ML4MD)
18	Lobna Saeed Abdelrazik Aly	adsorption of 5-fluorouracil, an anti cancer drug, at the surface of a natural zeolite
24	Jatin Kansal	SQuIRL: A Computed Infrared Spectra Database for Small Organic Molecules to Enable AI-Driven Spectroscopic Analysis
20	Salma Naimi	The Potential of γ-CuI as a Hole Transport Material: A DFT-Based Investigation
14	Aaron Gadzekpo	Linking sequence and properties in DNA-based materials through multiscale simulations and machine learning
22	Soumya Mondal	Unveiling Interactions of Peptide-bound Monolayer Protected Metal Nanocluster with Lipid Bilayer
26	Mariana Kozlowska	DNA Sequence-Controlled Biomolecular Assemblies for Synthetic Genomics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Effect of Nitrogen Incorporation in Amorphous HfO2

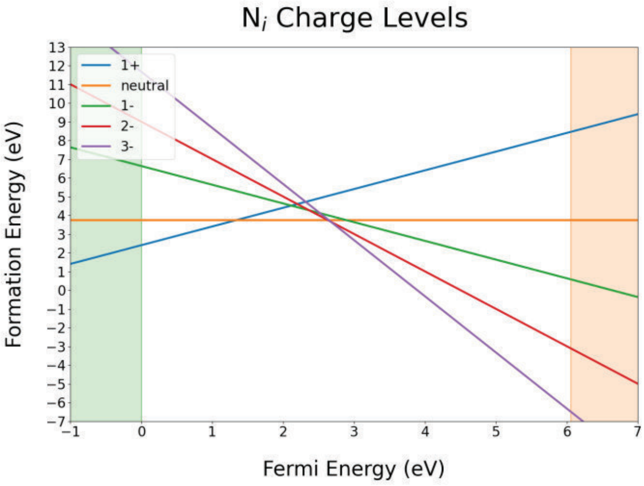
Isaac Mackley, Jack Strand, Alex Shluger

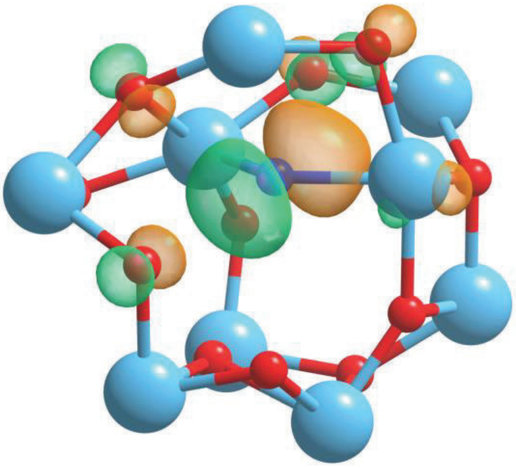
Department of Physics and Astronomy, University College London

The nitridation of HfO2 has demonstrated improvements in leakage current, bias temperature instability, and mobility of films. However, experimental studies have shown that the improvements are only at low nitrogen concentrations and that at higher concentrations performance is degraded.

This study aims to investigate the mechanisms underlying the negative aspects of nitridation by examining different nitrogen species within hafnia, including N, N2, and NH. We explore the charge states, geometries, charge transition levels (CTLs), and mobility of these species, highlighting their impact on the material's electronic behaviour. Our results show that while molecular nitrogen (N2) is thermodynamically more stable, its higher CTLs make it a less desirable defect, potentially detrimental to device performance. The study also examines defect reactions and interactions, revealing the formation of N2 as energetically favourable, with the largest energy gains occurring when two N interstitials combine. These findings offer insights into the defect landscape of HfO2 and provide guidelines for mitigating the negative effects of nitrogen incorporation in semiconductor devices, particularly in relation to leakage currents and electron tunnelling.

To carry out this computational work, CP2K is used to perform Density Functional Theory calculations. Non-local functionals are used to provide more accurate values for the band gap allowing for better analysis of the electronic structure of defects.





Probing Ultrafast Dynamics in Battery Cathodes with Automated Workflows

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Electrochemical energy storage in batteries is critical for the future energy economy, requiring systems that offer high energy density, rapid charging capabilities, and environmental compatibility. A key process in battery operation is the movement and localization of electronic charge, which has been extensively studied over timescales ranging from nanoseconds to seconds. However, our understanding of ultrafast electronic dynamics—occurring on femtosecond to picosecond timescales—remains limited, impeding insights into critical phenomena such as electron transfer, localization, and structural transformations in electrode materials like $LiMn_2O_4$ (LMO), despite their significant impact on battery performance [1].

In this talk, I will present our ongoing project, which investigates the formation and transport of electron polarons, with a particular emphasis on small Jahn-Teller polarons characterized by strong electron-lattice coupling. Using Density Functional Theory (DFT) simulations with hybrid functionals, where the fraction of exact exchange was tuned to calculations in the GW approximation, we aim to elucidate the fundamental processes governing charge localization and the structural transformations underlying Jahn-Teller polarons in LMO.

I will also introduce our approach to analyzing these ultrafast phenomena using automated workflows, which are essential due to the large data volumes and the complexity of the computational techniques involved [2]. To simplify this task, we have recently developed PerQueue [3], a modular and dynamic Python-based workflow manager designed to facilitate complex autonomous workflows. PerQueue's modular architecture supports dynamic capabilities, allowing the definition of workflows upfront and representing them as acyclic dependency graphs—even when dynamic processes are involved. This feature is vital when integrating DFT simulations with machine learning or Monte Carlo techniques. We aim to establish PerQueue as a foundational tool for managing complex, automated workflows in the study of battery cathode materials.

References

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AB INITIO STUDY OF POINT DEFECTS IN TUNGSTEN METAL

AMOL VERMA, NEERAJ MISHRA, GUY MAKOV

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Abstract

Point defects generated from radiation damage in tungsten (W) metal were studied using density functional theory (DFT). The energetics of vacancy defects, including single, di-, and tri-vacancies, and interstitial defects at tetrahedral and octahedral sites were calculated in W. We found that the adjacent di-vacancies were energetically preferred over separated vacancies, with a binding energy of 0.35 eV. Additionally, the interstitial defect at the tetrahedral site was energetically more stable than at the octahedral site. The material properties, including cell parameters, cohesive, and binding energies, were determined using two approximation methods: Local Density Approximation (LDA) and Generalized Gradient Approximation (GGA). The results obtained from the GGA method were relatively close to the experimentally reported values.

We calculated the formation energy for tri-vacancies in three configurations, including collinear vacancies along the diagonal and two non-collinear cases. We found that the collinear tri-vacancies were energetically preferred over other configurations.

Moreover, migration energies of point defects were calculated using the constrained relaxation method along the (001) direction. The migration energy of the vacancy defect was found to be a few meV and shows good agreement with experimental and previous theoretical results. Therefore, we conclude that vacancy defects can accumulate and form vacancy clusters in W during the radiation damage.

Modeling exciton dynamics on WS_2 monolayers under inhomogeneous strain from first principles

Amir Kleiner, Sivan Refaely-Abramson

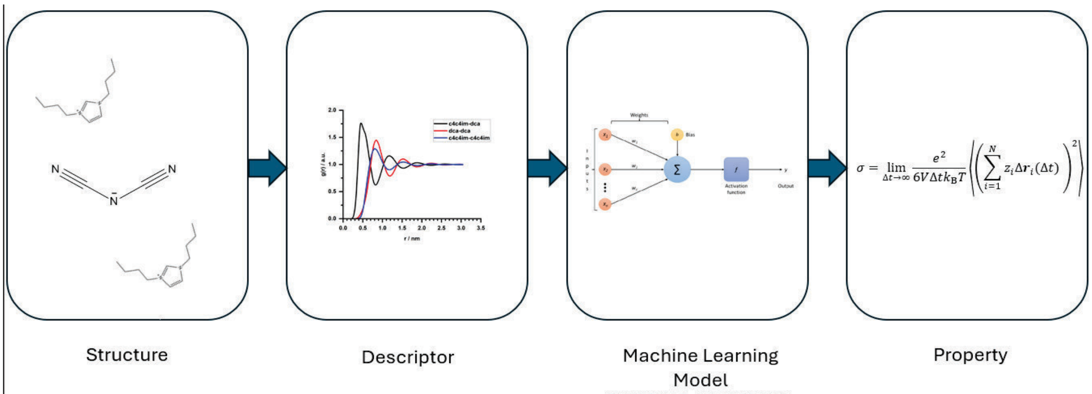
Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science, Rehovot, Israel

Monolayers of transition metal dichalcogenides (TMDs) are semiconducting materials that exhibit strongly bound long-lived excitons. The applicability of TMDs to physical devices depends on the ability to control the flow of energy and charge carriers in these materials. Since excitons are an electrically neutral species, strain gradients have been utilized to induce and control their flow.

In this work, we simulate the time-evolution of exciton distributions excited within an inhomogeneously-strained TMD monolayer by solving their equations of motion while evolving on a potential surface computed by first-principle methodologies. We investigate the effect of various strain profiles and initial conditions of the exciton distribution on the resulting dynamics. Our results offer insights into the physical origins of the strain-induced drift and diffusion exciton dynamics and allow the drawing of strain engineering design principles.

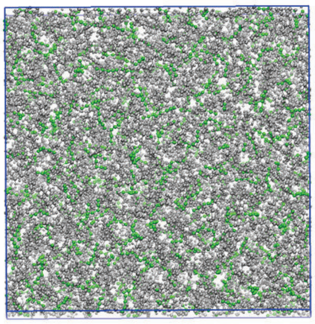
Predicting The Ionic conductivity From the Structure of Ionic Liquids with the Help of Machine Learning

Contributors: David Bienek

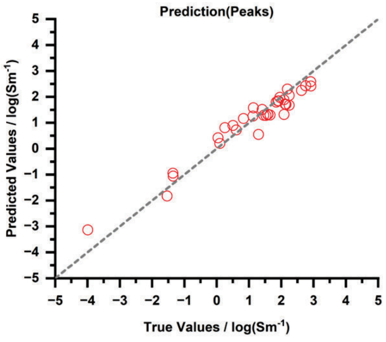


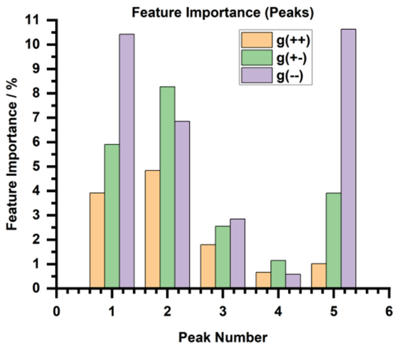
Çakir, M.; Cinarer, G., *International Research in Engineering Sciences III*, **2022**, *205-226*

This idea is based on a paper finding a connection between th hydrodynamic behaviour and structure of ionic liquids(D. Diddens, A. Heuer, J. Chem. Phys., 2023, 158, 154112). The idea was taken further to try to predict the ionic conductivity of ionic liquids with the help of machine learning models. Ionic liquids are relatively simple systems which make for a good environment to learn to work with machine learning models. Meanwhile machine learning models could help us better understand the connection between the structure and dynamic properties.



Since ionic liquids only consist of anions and cations, it was easy to construct a database of simulated systems by combining anions with cations. The structure was described through the radial distribution function, while the ionic conductivity was chosen as the property to predict. As for the machine learning models, random forest models, linear regression and neural networks were chosen for the prediction.





After the initial results, the quality of prediction was improved by refining the input data. Using the logarithm of the RDF, using only peaks from the RDF and using convolutional neural networks were all trialled to see what changes improve the results, as well as to why those changes improve the prediction. This was helped by the feature importance obtained from the random forest model.

In the end, the simple linear regression model only using the peaks of the RDF as an input proved to be the best model to predict the ionic conductivity of ionic liquids. This shows that it is important to not only understand and choose the right way to represent the input data, but also to not overlook simpler models in favour of more flashy ones. The knowledge from testing these machine learning models could also be helpful for others wanting to learn how to best use machine learning models for themselves.

Machine-learning-driven modelling of amorphous and polycrystalline perovskite systems

Laura-Bianca Pasca, Yuanbin Liu, Andy S. Anker, Ludmilla Steier, Volker Deringer

Recently, chalcogenide perovskites, most notably $BaZrS_3$, have gained attention as promising lead-free alternatives to the widely known hybrid halide perovskites. [1,2].

The growth of these polycrystalline films, typically starting from an amorphous precursor, has been studied with advanced experiments which provide local insights into the atomistic structure [3,4]. While computational studies have mainly focused on the bulk crystalline phase of $BaZrS_3$ [5], the polycrystalline nature of the synthesised material presents challenges for realistic modelling with ab initio methods.

With this issue in mind, we introduce a machine-learned interatomic potential (MLIP) for the emerging optoelectronic $BaZrS_3$ system, capable of describing both amorphous and polycrystalline phases with complex grain boundaries. We show how such a multi-purpose potential can be developed for applications in polycrystalline systems, using a de novo approach. Using MLIP-driven simulations, we quantify grain-boundary formation energies and create realistic simulations of nanoscale polycrystalline structures with different grain sizes. These simulations are directly comparable to experimental data, such as X-ray diffraction patterns and pair distribution functions.

This approach bridges the gap between atomistic modeling and experimental observations, paving the way for device-scale simulations of emerging optoelectronic and photovoltaic materials. We use $BaZrS_3$ as an initial test case, with the intent of extending the work to more complex perovskite systems, such as mixed-anion or -cation hybrid perovskites.

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The Zintl–Klemm Concept in the Amorphous State: A Case Study of Na–P Battery Anodes

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Elemental phosphorus has emerged as a promising anode material for sodium-ion batteries, offering a high theoretical capacity of 2596 mAhg⁻¹ in its fully sodiated Na_3P phase [1]. Among its allotropes, black phosphorus and amorphous red phosphorus have been extensively studied, often in composite form with conductive carbon materials to enhance cycling stability [2]. Notably, amorphous Na–P phases are commonly observed as intermediates during cycling, yet their structural evolution and role in sodium storage remain poorly understood.

The Zintl–Klemm concept has long been used to explain and predict the bonding and structures of crystalline solid-state materials [3]. In this work, using first-principles simulations combined with state-of-the-art machine-learning (ML) methods, we provide atomic-scale insight into the structural and energetic behaviour of amorphous Na–P phases. Our simulations are based on the MACE architecture for fitting message-passing ML interatomic potentials [4]. Subsequent analyses reveal the applicability of Zintl–Klemm rules in the amorphous state.

References

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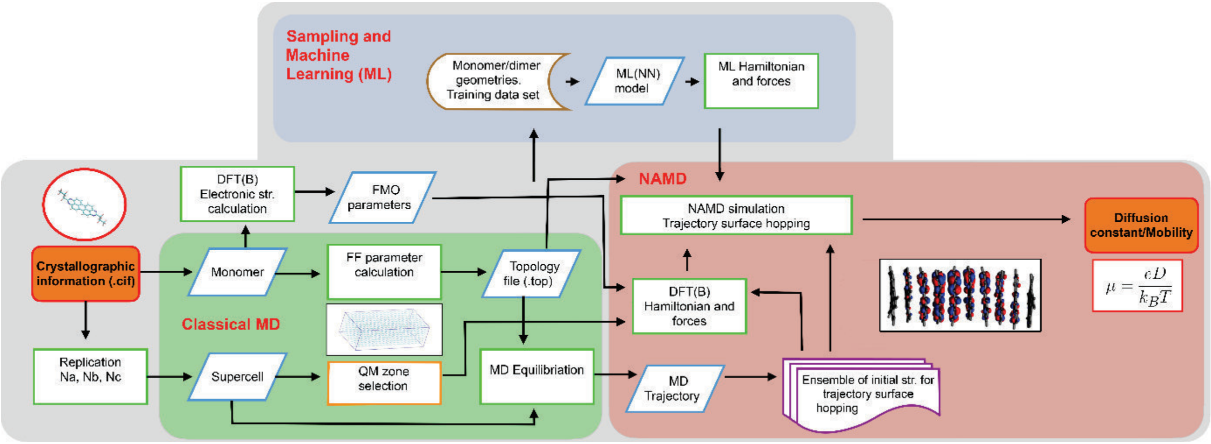
The calculation of intrinsic charge mobilities in organic semiconductors is a complex, multifaceted process. It involves several critical steps, including classical molecular dynamics (MD) simulations for system preparation, manual computation of reorganization energy, non-adiabatic simulations to evaluate transfer integrals, followed by production runs and simulations to ultimately determine charge mobilities.

To address these challenges, a workflow is under development to automate this entire process. The objective of this software is to simplify the complexities associated with the simulation chain, facilitating the calculation of key properties essential for assessing the viability of newly discovered organic semiconductors. To carry out these calculations, the crystal structure of the molecule to be analyzed is required as the foundation for the simulations. Additionally, the system is designed to handle large datasets, enabling the calculation of charge mobilities for numerous molecules to support the training of neural networks.



Classical and machine learning force fields for carbon dioxide

P. Strazzanti, I. Vacante, G. Calogero, D. Ricciarelli, I. Deretzis, A. La Magna, and G. Fisicaro

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Abstract:

Force fields have proven to be essential tools for studying molecular properties of various compounds like carbon dioxide (CO_2). Classical force fields describe interatomic interactions using classical equations, enable accurate simulations at a lower computational cost. Many force fields have been extensively developed for CO_2 (such as EPM2 [1,3] and TraPPe [1,3]) to describe thermodynamic characteristics or different non-covalent interactions between CO_2 molecules, including van der Waals forces, hydrogen bonding (H-bond acceptor), and electrostatic effects like instantaneous dipole-induced dipole and quadrupole-quadrupole interactions. Recently, driven by higher data availability and powerful high performance computers, a new class of precise and efficient interatomic potentials, such as machine learning interatomic potentials (MLIPs), emerged. This approach marks a paradigm shift, replacing physics-based functional forms of potentials with highly complex mathematical forms based on neural networks. These networks, trained on reference ab-initio datasets, can reproduce high-level quantum mechanical calculations with negligible errors, achieving accuracies comparable to experimental uncertainties. In the present study we assess the accuracy of classical and machine learning force fields, the latter represented by available interatomic potentials foundation models [2], for different phases of CO_2. We performed extensive validation studies of properties, including bond lengths and angles, vibrational features (zero-point energy, asymmetric and symmetric stretching), density, viscosity and diffusivity. Results have been compared to ab-initio and experimental data.

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Ab-Initio Investigation of the Aqueous Nafion-Platinum Interface for Enhanced PEM Fuel Cell Performance

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Proton exchange membrane fuel cells (PEMFCs) are among the most promising technologies for clean energy applications, relying on platinum (Pt) as the primary catalyst. The interaction between Nafion, the widely used polymer electrolyte, and Pt at the electrode interface plays a crucial role in the performance and durability of these fuel cells. While previous studies have focused on the macroscopic properties of Nafion, a detailed atomistic understanding of its interaction with Pt, particularly in the presence of water, remains incomplete. The interfacial behavior, proton transport, and electronic structure modifications induced by the electrolyte environment require further exploration through ab-initio methods [1-3].

In this study, we employ density functional theory (DFT) calculations to investigate the structural, electronic, and chemical properties of the Nafion-Pt interface in an aqueous environment. Our model incorporates explicit water molecules to simulate the solvation effects, providing a more realistic representation of the interface. We analyze charge transfer, adsorption energies, and electronic structure changes induced by hydration. Furthermore, charge density difference (CDD) analysis and projected density of states (DOS) calculations reveal key insights into the interaction between the polymer's sulfonic acid groups and the metal surface [4-6].

Our findings indicate that the presence of water significantly modifies the interfacial properties, enhancing the proton-conducting ability while altering the electronic states of Pt. The results contribute to a deeper understanding of catalyst degradation mechanisms and may guide future improvements in PEMFC performance through optimized electrode-electrolyte interfaces.

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Advances in CO_2 Reduction Using MOFs: A Computational Approach

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Department of Physics, Indian Institute of Science, Bangalore, 560012, Karnataka, India

Reducing carbon dioxide (CO_2) emissions is essential for addressing climate change and achieving a sustainable carbon economy. Metal-organic frameworks (MOFs) have emerged as promising materials for CO_2 capture due to their high specific surface area and tunable pore structures. A computational approach is used to identify and design MOFs with high selectivity for CO_2 capture and separation from gas mixtures. We used grand canonical Monte Carlo (GCMC) simulations to investigate the adsorption isotherms for various gas mixtures within prominent MOFs, including IRMOF-1, HKUST-1, ZIF-8, ZIF-6*, and qMOF-*. Analyzing these isotherms allows for the identification of structures demonstrating optimal CO_2 adsorption. Our simulations give a deep insight into the gas adsorption mechanisms by investigating the intermolecular interaction between the nodes and the adsorbate. Furthermore, generative AI models will be used to design novel MOF structures, predicted to demonstrate enhanced gas separation capabilities. These proposed structures will then be validated through computational simulations to assess their performance against targeted gas mixtures. This approach, integrating statistical mechanics with AI-driven design, aims to streamline the discovery of advanced MOFs, providing a scalable pathway for developing materials with optimized separation efficiencies.

*Corresponding author: maiti@iisc.ac.in

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Integrating Workflows, HPC, and Domain Packages for Materials Science: a closer look at TextS

Rodrigo Cortes Mejia, Marvin Müller, Nikolai Pfisterer, Sruthy Sreenivasan and Ivan Kondov

Materials science simulations is not only a complex area of knowledge, but it can also face multiple challenges due to intricate workflows, efficiency of use of computational resources, as well as reuse and extension of code and data. The Python-based TextS and TextM domain specific languages, DSL simplify the full life cycle of modeling, simulation, and data analysis in materials science by integrating workflow, workload, and storage management systems, thus alleviating these issues [1].

The tools provided as part of TextS and TextM facilitate the construction, parsing, interpretation, syntax and semantic check, execution, evaluation, and extension of models. For example, integration of database storage as part of the workflow system ensures the provenance and persistence of data, while different execution modes and transparent HPC interface help to optimize the use of computational resources. Both DSLs provide support for various data types and structures, as well as physical units, contributing to their reuse value. Additionally, TextM works as interface to domain-specific computational packages with support for automatic job submission, data collection, and visualization. The present contribution provides a closer look at the tools and features of TextS and TextM, as well as practical uses for Material Science.

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Coherence locking in a parallel NMR probe defends against gradient field spillover

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Abstract

The implementation of parallel nuclear magnetic resonance detection aims to enhance measurement throughput in support of high throughput screening applications including, for example, drug discovery. In support of modern pulse sequences and solvent suppression methods, it is important that each detection site has independent pulsed field gradient capabilities. Hereby, a challenge is introduced, in which the local gradients applied in parallel detectors introduce field spillover in adjacent channels, leading to spin dephasing and hence to signal suppression. This study proposes a compensation scheme employing optimized pulses to achieve coherence locking during gradient pulse periods. The design of coherence-locking pulses utilizes optimal control to address gradient-induced field inhomogeneity. These pulses are applied in a PGSE experiment, and a parallel HSQC experiment, demonstrating their effectiveness in protecting the desired coherences from gradient field spillover. This compensation scheme presents a valuable solution for magnetic resonance probes equipped with parallel and independently switchable gradient coils.

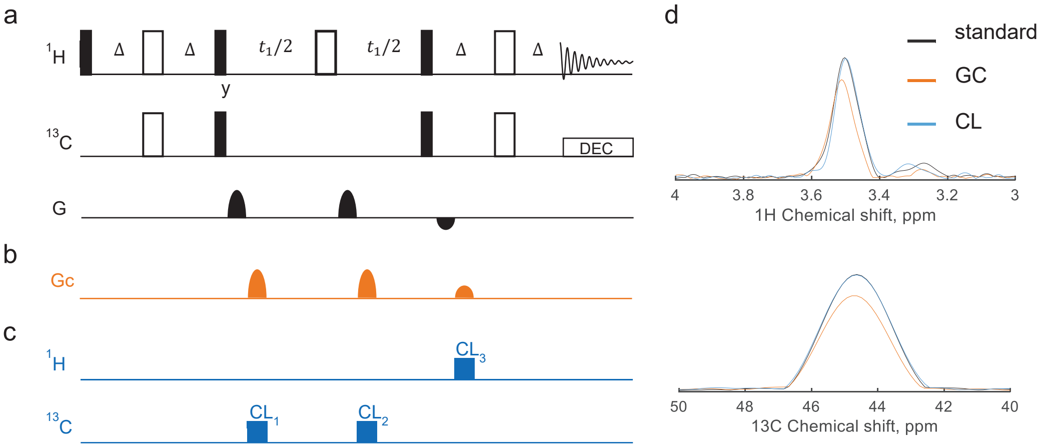

Figure 1. View of the three experimental HSQC scenarios. (a) The standard HSQC pulse sequence, in which the gradient pulse ratio is set to 2 : 2 : −1 to select the S+ → S+→ I+ → I− coherence pathway. (b) Additional gradient pulses from a second detector, set at a ratio of 2 : 2 : 1, are incorporated into (a) as coupled gradients. (c) Coherence locking pulses are introduced to (a), aligned with the coupled gradient pulses. Specifically, CL_1 and CL_2 are applied to ^{13}C, while CL_3 is applied to ^1H. (d) The 1D projected spectra corresponding to the three experimental scenarios, obtained using 0.6 M glycine in D_2O.

Enhancing the Lifetime of Triplet Excitons Through Controlled Intermolecular Interactions

Abstract

Singlet fission (SF) is a process in which a singlet exciton is converted into two triplet excitons, significantly enhancing charge generation in organic solar cells. It has been shown that the rate of SF and the lifetime of the generated triplet excitons strongly depend on the molecular arrangement. In this work a cofacial orientation of pentacene molecules is achieved by embedding organic linkers containing pentacene in a surface-anchored metal-organic framework. Transient absorption spectroscopy and a quantum mechanical analysis have been used to analyze the exciton dynamics in a broad spectral range from near-ultraviolet to near-infrared. The observed spectra indicate that a singlet excited state generates a correlated triplet pair within a few picoseconds. Subsequent dynamics show the formation of long-lived excitons (39 μs) with triplet character. This exceeds by far the observed lifetime of triplet excitons generated in pentacene thin films and may enhance triplet exciton harvesting capabilities in photovoltaic cells.

Atomic Structure of Amorphous $Ge_2Sb_2Te_5$: Machine Learning Potentials and Hybrid Reverse Monte Carlo Simulation

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Phase-change materials (PCMs) such as $Ge_2Sb_2Te_5$ (GST) are central to next-generation non-volatile memory and photonic applications due to their rapid switching capabilities and stable data retention[1]. A detailed understanding of their atomic structure is crucial for technological advancement[2].

Here, we present an innovative approach that integrates machine learning potentials with hybrid reverse Monte Carlo (HRMC) simulations[3] to construct an energetically-stable, experimentally consistent model of amorphous GST. By combining experimental X-ray scattering data with energetic stability assessments, our method effectively resolves the longstanding slight discrepancy between simulation and experiment and overcomes the limitations of traditional reverse Monte Carlo methods that lack energy consideration[4].

Looking ahead, these insights into medium-range order and atomic-scale dynamics are expected to guide predictive models that help to understand the mechanisms of resistance drift based on structural relaxation, addressing key challenges in PCM device performance.

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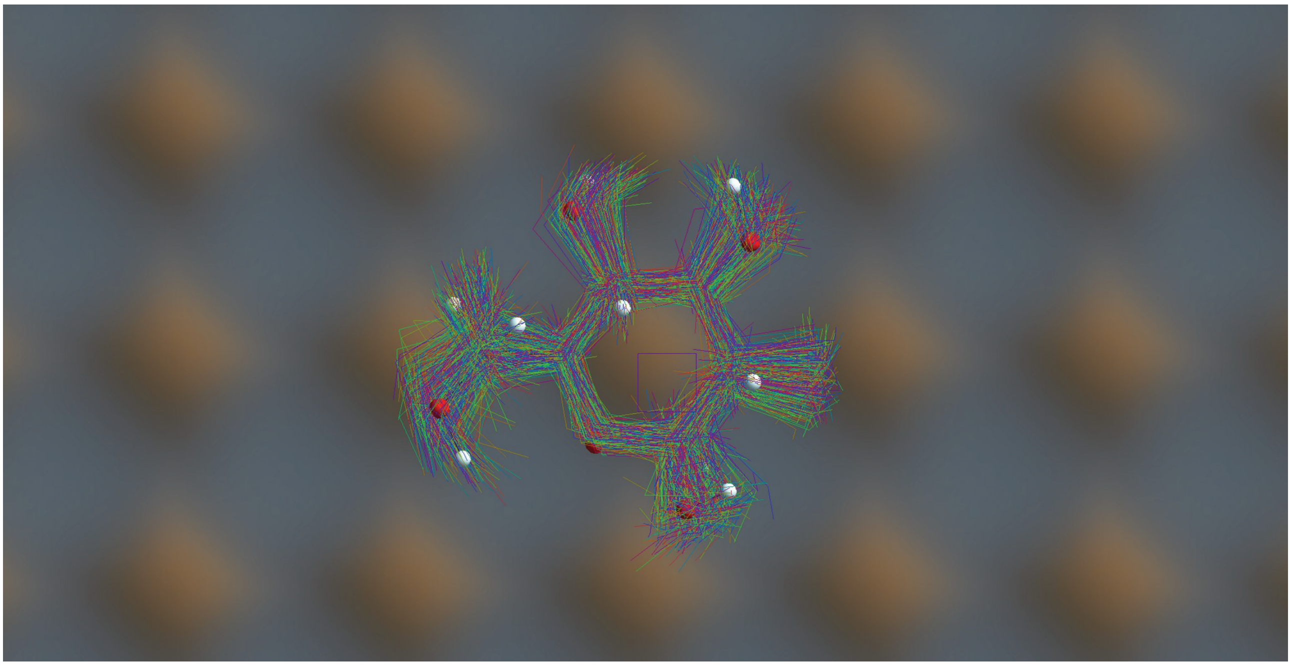
Efficient Exploration of Phase Space for Organic Molecules on Ionic Crystal Surfaces using FireCore and GPU Acceleration

The design and simulation of organic molecules on ionic crystal surfaces, rather than in solution, allow for the creation of functional structures tailored to specific surfaces. This approach enables the precise design of novel materials by understanding how molecules interact with and organize on well-defined surfaces. We present a computational method using the FireCore program, leveraging GPU acceleration to parallelize simulations and rapidly sample the phase space of organic molecules. By running hundreds of replicas on a single GPU, we demonstrate the capability to efficiently explore the degrees of freedom of these molecules on surfaces. Our method involves calculating forces and energies, which will be used to compute free energies via thermodynamic integration and free energy perturbation methods. This approach enables the prediction of how molecules behave, contributing to the development of novel useful structures with tailored functionalities. Our work demonstrates the potential of advanced computational tools to enhance materials design workflows through efficient phase space exploration.



Deep learning assisted investigation of drug-carrier interactions using drying droplet patterns

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Deep learning provides a powerful tool for studying the interactions between biomaterials by analyzing their drying droplet patterns. Traditional available techniques, such as Circular Dichroism (CD) spectroscopy, fluorescence spectroscopy, and mass spectrometry are costly and time consuming causing a limitation in their capacity to do high-throughput interaction screening. Previous research has successfully utilized deep learning models to classify biomaterial interactions with high accuracy including histone-DNA complexes[1], protein-immunoglobulin[2] and amyloid beta mutants[3]. This research aims to utilize convolutional neural networks (CNNs) to predict the drug-carrier binding affinity. In this study, Human Serum Albumin (HSA) was used as a carrier along with various drugs. Drug-carrier mixtures were pipetted onto hydrophobic glass surfaces, followed by imaging their drying droplet patterns using polarized light microscopy (PLM). These images were used to train CNN models to classify the binding affinity as validated by complementary techniques such as CD (**Figure 1**). The trained model was tested on new unseen drugs to predict their binding affinity to HSA, followed by verification of the prediction with experimental data. This method has great potential as a high-throughput screening tool for optimal drug-carrier combinations.

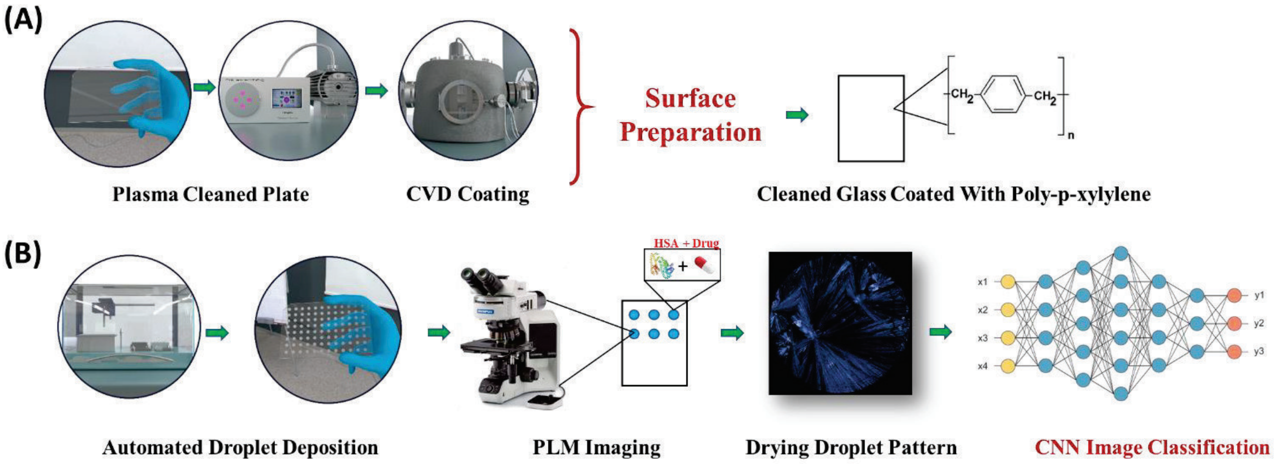

Figure 1. Schematic Diagram of the procedures followed for the classification of Carrier-Drug interactions. **(A)** Surface preparation of glass substrates including plasma cleaning and coating with poly-*p*-xylylene using CVD (Chemical vapor deposition) before droplet deposition. **(B)** Automated droplet deposition under controlled conditions before imaging the droplets using a PLM (Polarized Light Microscope). CNN (Convolutional Neural Network) was trained on PLM images for classifying Carrier-Drug interactions.

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A Hierarchical Variational Autoencoder for Polymer Design using Fused Latent Representations

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Abstract

Variational Autoencoders (VAEs) have emerged as efficient generative models for polymer structure design. They enable a smooth exploration of the molecular space through a continuous latent space. However, current VAE-based methods [Dai et al., ICLR (2018)], [Jiang et al., npj Comput Mater 10, 139 (2024)] often rely solely on topological and chemical composition information to encode the input polymer into a relevant fingerprint. They neglect Euclidean features such as 3D atomic coordinates and inter-atomic distances which are crucial for the calculation of polymer properties like density or refractive index. This limitation hinders the training of subsequent property regression models fed by the VAE-based fingerprint.

To address this issue, we propose a novel VAE architecture leveraging two distinct encoders. First, a hierarchical variational autoencoder (HierVAE) [Jin et al., ICML (2020)] encodes the intricate topological and chemical information of the polymer. Second, a pre-trained neural network potential (NNP) model generates polymer embeddings that incorporate 3D Euclidean features. Then, we introduced an attention mechanism and a multi-layer perceptron (MLP) to fuse these two representations for creating a richer and unified polymer feature embedding.

We trained the dual encoder on the St John et al. dataset [J. Chem. Phys., 150, 234111 (2019)]. The attention mechanism aggregates the NNP model embeddings to a fixed size to be compatible with the HierVAE decoder. Inspired by the work of Mao et al. [Digit. Discov. 2, 1098-1103, (2023)], the fused polymer representation is transformed into a discrete representation using the Gumbel-SoftMax trick [Jang et al., ICLR (2017)] and subsequently used to train a Factorized Machine (FM) model [Rendle et al., ACM Trans. Intell. Syst. Technol., 3, 1-22 (2012)] for property prediction. The trained FM model weights are transformed into a QUBO (Quadratic Unconstrained Binary Optimization) matrix. Then we solve the QUBO using the Fujitsu's Digital Annealer (DA) [Aramon et al., Frontiers in Physics 7 (2019)] to compute the optimal bit vector configuration associated with optimal property values. We feed the VAE decoder with the optimal bit vector to generate novel polymers with desired properties.

We used our dual encoder architecture to generate richer polymer binary vector representations. Such improved fingerprints, including topological, chemical and Euclidean information, resulted in a significant decrease of the FM model validation error. When applied to a dataset of polymer structure and molecular weight labels, the FM error, compared to using only the HierVAE encoder, decreased from 154 amu to 83.3 amu. The mean absolute percentage error (MAPE) also decreased from 22.2% to 11.9%. Furthermore, the subsequent property optimization using the FM-DA generated polymers with property values beyond the range observed in the training data, demonstrating the extrapolation capabilities of our method. These results demonstrate the effectiveness of incorporating 3D Euclidean features into the latent representation.

We proposed a novel architecture and methodology for polymer design by fusing topological, chemical, and Euclidean features from two independent encoders within a hierarchical VAE framework. This dual-encoder fusion approach offers a promising pathway for accelerated materials discovery and design, enabling the generation of novel polymers with targeted properties.

Linking structure and (chir)optical properties of self-assembling systems: A porphyrin-peptide conjugate as a case study

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Conjugation of porphyrin with peptides and proteins, inspired by Nature, has been proven to be a versatile strategy for forming higher order structures, which can be used to exploit the excellent structural, photochemical and electrochemical properties of the tetrapyrrole ring.[1,2] The introduction of chirality may affect aggregation and widens the applicability range of the systems, e.g. to asymmetric catalysis and chiral sensing.[3] However, controlling the structures of these assemblies is still challenging as it depends not only on the nature of the conjugates, but also on the solvent and on thermodynamic parameters, as well as on the specific assembly route employed. UV-Vis absorption spectroscopy and electronic circular dichroism (ECD) are sensitive to the organization of porphyrins, but the relationship between spectral observables and geometric arrangement of the chromophores is well-established only for relatively simple and regular structures. Here, taking 5(4'-carboxyphenyl)-10,15,20-triphenylporphyrin covalently linked to [1–12]magainin (GIGKFLHSAKKF)[4] in water as a case study, we investigate the relationship between aggregate structure and UV-Vis absorption/ECD spectra, using an approach that combines quantum mechanical exciton modeling[5] and all-atom molecular dynamics simulations with enhanced sampling methods. Suitable descriptors and dimensionality reduction techniques are used to correlate the spectra with the structure and chirality of the aggregates.

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Poster Title: *High-Throughput Computational Screening of Silanes for Tire Applications: Bridging Atomistic Simulations and Macroscopic Performance* (Master Thesis)

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Summary: We report the development and implementation of a multi-scale computational framework for the systematic screening of silane coupling agents for tire compound applications, with particular emphasis on optimizing the trio of critical performance parameters: rolling resistance, wet traction, and abrasion resistance. The methodology integrates classical molecular dynamics (MD) simulations with ab initio density functional theory (DFT) calculations to quantitatively characterize key molecular-level phenomena, including silica–silane interfacial energetics, filler–filler network mechanics, silane-polymer covalent crosslink stability, and Silane molecular diffusivity within heterogenous silica-polymer matrices. These nanoscale descriptors are hypothesized to correlate strongly with experimentally observed macroscopic tire performance metrics, specifically the nonlinear viscoelastic response (Payne effect) and mechanical wear resistance profiles under dynamic loading conditions. Chemical space exploration encompasses approximately ~18,000 silane structures curated from PubChem, after being subjected to preliminary filtering protocols based on established tire industry application criteria and toxicity constraints. The resultant observables derived from our MD and DFT computational ensemble serve as the training corpus for a Gaussian Process Regression model framework, which subsequently facilitates a Bayesian optimization-mediated active learning protocol. This iterative approach enables efficient navigation of the vast chemical landscape while minimizing computational expense through strategic sampling methodologies. The fundamental scientific inquiry addresses the feasibility of predicting silica–silane interfacial properties—and by extension, related molecular descriptors crucial to performance—via an active learning paradigm that optimizes the simulation-to-insight ratio. Workflow automation and reproducibility are ensured through implementation within the Automated workflows for computational science (AiiDA) framework, providing complete provenance tracking and computational governance throughout the pipeline.

Insights into modeling polymers with Machine Learning Interatomic Potentials using model systems

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During the past years Machine Learning Interatomic Potentials (MLIPs) have gained wide popularity across the molecular dynamics (MD) simulation community. The most recent developments, including equivariant and graph based models like NequIP, MACE or GRACE, have pushed the boundaries of MD simulations to new limits. For instance, these approaches enable calculations for millions of atoms and arbitrary number of chemical species with quantum chemical accuracy and calculations of full phase diagrams within hours or days instead of months or years.

Nearly all of these types of potentials have in common that they only rely on information about atom positions and chemical species, but do not include explicit topological information. Despite the fact that this enables chemical reactions, such topological information might be especially relevant in large molecules like polymers. For example relaxation processes are governed by the topology of polymers, and furthermore, long time scales of simulation are needed to characterize them. Local short-ranged descriptors, like in the Atomic Cluster Expansion (ACE), can not take into account long-ranged interactions that rely on the topology.

Because simulating polymers requires large systems with many hundreds of atoms, performing accurate quantum chemical reference simulations is difficult. Approximations like Density Functional Theory (DFT) may influence the behavior of polymer systems in an unpredictable manner and are still to expensive for simulations of long timescales. Thus, it is not possible to compare a trajectory which was created using MD and MLIPs to a proper reference trajectory, created from ab initio MD. A direct consequence of this is that we cannot distinguish between effects of DFT and the fitted MLIP.

Instead, we use model systems (which can be computed with traditional MD) as the ground truth and fit MLIPs to these model systems. Starting with dimers, and extending to longer chains later, we investigate how accurate polymers can be modeled using MLIPs with short-range descriptors. Besides energy and force errors, for example the mean squared displacement of monomers can be seen as a good indicator for the quality of a fit, since it shows subdiffusive behavior for long timescales. In particular, we are also interested whether the fitted MLIPs are able to represent the interactions of atoms at the chain ends correctly. For instance, we investigate how well the MLIP can discriminate between interactions with a directly bonded atom from the same chain and non-bonded atoms of the same or other chains, which are very close. Also effects of temperature may be investigated in this study. It is well-known that structures generated during MD simulations are temperature-dependent. Thus, it is unclear if a MLIP, trained on structures generated at a certain temperature, can be used to run MD simulations at other different temperatures. We shed light onto this question using model systems.

Title:

Linking sequence and properties in DNA-based materials through multiscale simulations and machine learning

Contributors:

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Abstract:

DNA can be used as a sequence-programmable building block for materials with complex properties and behaviours. We present ongoing research aimed at accelerating the development of DNA-based materials through multiscale simulations, aided by machine-learning-based parameter optimisation. One class of such materials is condensates of small DNA molecules, typically with three to six arms, that form networks via hybridisation. The sequence-encoded properties of these so-called DNA nanomotifs translate into mesoscopic phase behaviour and responses to heat, mechanical, or molecular stimuli. We present models of nanomotif-based materials at different scales, with a focus on Bayesian optimisation as a tool to transfer information between scales. In combination with experimental validation, such strategies can facilitate the scale bridging required to utilise sequence-property relationships for applications in biomimetic systems or DNA-based computing.

Philipp Dullinger, Niklas Kappel, Joshua Futterer, Wolfgang Wenzel

Machine learning for Molecular Dynamics Simulations (ML4MD): A divide-and-conquer approach towards accurate, transferable and fast model for virtual materials design by classification

Virtual materials design is strongly dependent on an accurate description of the systems of interest beyond just single molecules – here complexity arises both from the environment and the fact that several properties are dynamic in their nature: chemical reactions in solution and in heterogeneous catalysis comprise just some examples of this. Molecular Dynamics (MD) simulations, permit the treatment of such systems.

In principle ab-initio/first principle methods can be used to describe the intermolecular interactions needed. However, with a first-principles approach the time scales reasonably reachable in ab-initio quantum chemistry calculations are so short, that at best model systems can be addressed. Opposed to that, classical force-field molecular dynamics, permit the treatment of systems on timescales which are more than 100,000 times longer. But for rare events even this improvement is insufficient for direct sampling. Instead "advanced sampling methods" are then used to additionally bias systems into the desired regions of phase space.

While classical force fields work well for certain applications, it is generally acknowledged that they will fail for cases for which they haven't been parameterized - be it far from the equilibrium geometry or during chemical reactions.

In order to overcome these problems, there has been a decade-long effort to use machine learning (ML) methods to go beyond the limits of classical force fields, while maintaining a speed advantage over ab-initio methods.

Here we present a novel alternative approach, where we partition our system into individual parts described as graphs.

This is done by a first classifier and yields a decomposition into classical long-range parts and short-ranged parts, which can use any desired ground-truth DFT/ML/…

Another classifier decides when the latter actually needs to be evaluated and when we can use a simpler method. For this we also suggest a transferable scheme, for approximating it by a classical expression.

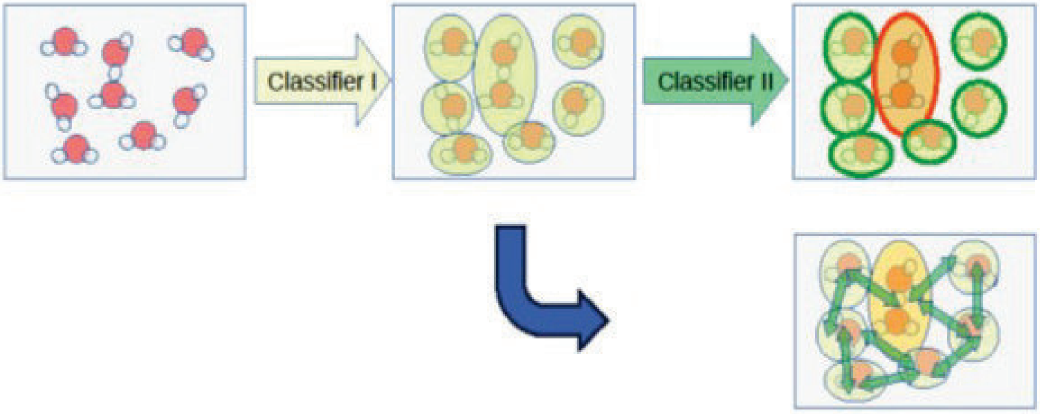

Figure 1: Sketch of Classification & Networks. A first classifier converts the conformation into graphs which mostly, but not exclusively correspond to covalently bound molecules. A second classifier decides which intra-graph interactions are treated by the intra-graph model and which need to be treated by the QM-ML model. The inter-graph interactions are evaluated by an interaction model, which generalizes expressions similarly used in classical force fields.

5-Fluorouracil (5-FU) is a widely used anticancer drug that exerts its cytotoxic effects by inhibiting thymidylate synthase and disrupting nucleic acid synthesis. However, its clinical efficacy is often limited by drug resistance and systemic toxicity. Recent advancements in drug delivery systems have explored the potential of zeolites—microporous aluminosilicate materials—as carriers for controlled and targeted drug release. Zeolites provide a unique framework for enhancing 5-FU stability, prolonging its release, and improving its bioavailability, thereby reducing side effects and enhancing therapeutic outcomes. Moreover, their well-defined microporous structures and ion-exchange properties make them valuable for studying the adsorption, stability, and molecular interactions of 5-FU in different environments.

In this work, we investigate the interaction of 5-FU with various cation-exchanged clinoptilolites, a natural zeolite, using a combination of force-field methods, molecular dynamics simulations, and density functional theory calculations. Through these approaches, we determine the adsorption energies of different molecular configurations and identify which cation-exchanged zeolite provides the most favorable adsorption properties for 5-FU.

The Potential of γ-CuI as a Hole Transport Material: A DFT-Based Investigation

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Perovskite solar cells (PSCs) hold great promise for next-generation photovoltaics due to their remarkable efficiency and cost-effectiveness. However, the reliance on organic Hole Transporting Materials (HTMs) remains a major limitation, as these materials are costly and contribute to perovskite layer degradation, hindering long-term stability and commercialization. This study explores γ-CuI as a potential inorganic HTM through first-principles calculations within the Density Functional Theory (DFT) framework. Using both the Generalized Gradient Approximation (GGA) and GGA + Hubbard correction, we assess its structural, mechanical, electronic, and optical properties. Geometry optimization confirms its stability, while mechanical analysis suggests suitability for flexible PSCs [1].

Electronic and optical investigations reveal that γ-CuI exhibits a high refractive index and low extinction coefficient across the visible and infrared spectra, with minimal reflectivity and absorption, key attributes for efficient light management in PSCs [1].

The results highlight γ-CuI as a strong candidate for replacing organic HTMs, offering improved stability and cost-efficiency for advancing perovskite solar cell technology.

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Unveiling Interactions of Peptide-bound Monolayer Protected Metal Nanocluster with Lipid Bilayer

Soumya Mondal , Dr. Tarak Karmakar*

Monolayer-protected atomically precise nanoclusters (MPCs) are potential candidates for drug delivery because of their unique, versatile, and tunable physiochemical properties. The rational design of nano-sized drug carriers relies on a deep understanding of their molecular-level interactions with cell membranes and other biological entities. Here, we applied coarse-grained molecular dynamics and umbrella sampling simulations to investigate the interactions between the Magainin 2 (MG2)-loaded Au144(MPA)60 nanocluster (MG2-MPC) and model anionic tumor cell membrane. Electrostatic interactions between MPC ligands and MG2's positively charged residues with the polar head groups of lipids play a crucial role in the adhesion of the MG2-MPC complex to the membrane surface. Furthermore, MG2-MPCs self-assemble in the linear trimeric supramolecular aggregate on the bilayer surface indicating a possible mechanism of MPC's action in peptide delivery to the membrane.

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SQuIRL: A Computed Infrared Spectra Database for Small Organic Molecules to Enable AI-Driven Spectroscopic Analysis

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One of the fundamental challenges in materials design is accurately determining the structure of synthesized compounds. Infrared (IR) spectroscopy is widely used for structural characterization. Existing spectral libraries are often incomplete, making it difficult to identify new molecular structures with confidence. Artificial intelligence (AI) and machine learning (ML) offer promising solutions for predictive spectral analysis, but their development is hindered by the lack of high-quality, large-scale training datasets.

To address this gap, we present a comprehensive computational IR spectra database covering approximately 134,000 small organic molecules. The optimized molecular geometries are derived from the QM9 dataset [1,2], while the IR spectra are computed using the wB97XD/Aug-cc-pVTZ [3-5] level of quantum chemistry. In addition to the spectral data, we provide a detailed statistical analysis of species; such as molecular complexity, frequency of functional groups or interatomic interactions present in the database. Furthermore, we compare IR spectra obtained from experimental references offering valuable insights into computational accuracy.

Our database provides a valuable foundation for AI and machine learning applications in spectral analysis, helping to build more accurate and reliable predictive models. The goal of this project is to make molecular characterizations more efficient and accessible, driving advancements in AI-driven molecular science.

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DNA Sequence-Controlled Biomolecular Assemblies for Synthetic Genomics

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The development of synthetic genomics technologies is an emerging field essential in life science and healthcare, including immunotherapy treatments or gene therapies for previously incurable diseases. Effective programming of DNA-sequence alterations and the *in-silico* prediction of DNA structure organization, the thermodynamic and mechanical properties, as well as interactions with other molecules, are of key importance for applications in novel DNA-containing materials for nanomaterial technologies and life science.

The development of a virtual pipeline for the analysis and simulation of DNA and DNA-containing biomolecular complexes that can help guide the synthesis of functional DNA sequences, as well as the understanding of the change in the DNA properties and assembly functionality upon specific modifications in the sequence, requires integrative multiscale approaches. The predictive machine learning trained on data obtained with scale-bringing approaches and active learning strategies could potentially enable efficient navigation towards DNA sequence programming and desired functional materials.

Here, we demonstrate molecular-based differences in DNA functionality and interactions with histones using nucleosome-level molecular dynamics simulations. Nucleosome dynamics govern DNA accessibility and chromatin function; therefore, understanding both local and large-scale genome organization – and how it changes due to diverse modifications, mutations, or specific conditions – is crucial for regulating processes such as gene expression, DNA replication, and cell division. We report DNA sequence-dependent interactions and differences in canonical and centromeric dynamic nucleoprotein complexes. Additionally, we demonstrate the potential of machine learning to transfer information between simulation scales used for assembling DNA fragments (i.e., DNA nanomotifs). Its computational power and predictive capabilities are presented in the context of integration into iterative design strategies for biomimetic applications, such as mechanically tunable biomaterials and information-processing platforms.

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Multi-scale Modeling of Ethylene Oligomerization on Ni-NU-1000: From DFT and GCMC/MD to Kinetic Mechanism.

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Ethylene oligomerization represents an important industrial process, and Ni-based MOFs have emerged as promising catalysts for this reaction [1,2]. A comprehensive understanding of the role of Ni activity and product diffusion in ethylene oligomerization is imperative for the optimization of MOF-based catalysts [3]. To this end, a multi-scale modeling approach is employed, integrating periodic and cluster density functional theory (DFT) calculations with energy corrections on cluster models and adsorption/diffusion studies with molecular dynamics (MD) and grand canonical monte-carlo (GCMC) to construct a comprehensive kinetic mechanism for Ni-NU-1000 catalyst.

Initially, periodic DFT is utilized to model the complete Ni-NU-1000 ethylene oligomerization mechanism and to furnish an initial estimate of reaction energetics. To enhance the accuracy of the model, a QM/QM correction scheme is employed, which refines reaction barriers while preserving the structural integrity of the catalyst [4]. Subsequently, the ethylene transport to active sites and product diffusion/adsorption within Ni-NU-1000 are investigated using MD and GCMC simulations.

The results of this study underscore the pivotal role of reaction energetics and adsorption/diffusion in determining catalytic efficiency. By using a multi-level theoretical framework, this study offers significant insights into the catalytic mechanism of Ni-based MOFs and emphasizes the importance of a multi-scale approach for realistic catalyst modeling. The methodology is not only applicable to Ni-NU-1000 but can also be extended to other MOF-based catalytic systems.

Literature

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