MM 20: Data Driven Material Science: Big Data and Workflows III

Time: Tuesday 10:15–13:00 Location: C 243

MM 20.1 Tue 10:15 C 243

Bulk and Surface Properties of cesium-telluride Photocathode Materials via High-Throughput Density Functional Theory Calculations — •Holger-Dietrich Sassnick[1] and Caterina Cocchi[1,2] — [1]Carl von Ossietzky Universität Oldenburg, Physics Department, 26129 Oldenburg, Germany — [2]Humboldt-Universität zu Berlin, Physics Department and IRIS Adlershof, 12489 Berlin, Germany

Cesium-based photocathodes such as cesium-telluride are commonly used as electron sources in particle accelerators but the lack of knowledge of their crystal structure and stoichiometry during synthesis hinders their control. To predict which compounds are more likely to form and to characterize their properties, we apply a high-throughput workflow based on density functional theory calculations. Firstly, we calculate the formation energies and electronic properties of bulk phases obtained from computational databases employing the meta-GGA functional SCAN, which is known to provide accurate results for these systems [Saßnick & Cocchi, *Electron. Struct.* **3**, 027001 (2021)]. Our results indicate that a large number of different crystal structures may form and coexist in actual samples [Saßnick & Cocchi, *J. Chem. Phys.* **156**, 104108 (2022)]. In a second step, surface properties, which play a fundamental role in the photocathode performance, are calculated for a selected set of stable bulk crystals. The studied surfaces exhibit diverse properties ranging from semiconducting to metallic character with the latter being formed by facets terminated with an excess of metallic species.

MM 20.2 Tue 10:30 C 243

Thermodynamic and phonon properties of multi-alkali antimonides from density-functional theory and machine learning — •Julia Santana-Andreo, Holger-Dietrich Sassnick, and Caterina Cocchi — Carl von Ossietzky Universität Oldenburg, Institute of Physics

Modern advancements in generating ultrabright electron beams have ushered in innovative experimental techniques in particle accelerators. However, the current challenge lies in improving the quality of electron sources primarily with novel photocathode materials, such as alkali-based semiconductors. In this work, we employ density functional theory combined with machine learning techniques to probe the thermodynamic stability of various alkali-based crystals, emphasizing the role of the approximations taken for the exchange-correlation (xc) functional. Our results reveal that SCAN offers the optimal trade-off between accuracy and computational costs to describe vibrational properties in these materials. Furthermore, it is observed that systems with a higher concentration of Cs atoms exhibit enhanced anharmonicities, which are accurately predicted and characterized with the employed methodology.

MM 20.3 Tue 10:45 C 243

Energetic and electronic properties of K-Sb and Na-Sb binary crystals from high-throughput ab initio calculations — •Richard Schier, Holger-Dietrich Sassnick, and Caterina Cocchi — Carl von Ossietzky Universität Oldenburg, Institut für Physik

The development of photocathode materials for the generation of ultrabright electron beams is essential for optimizing the performance of synchrotrons and thus to open unprecedented opportunities to access the fundamental properties of materials. Alkali-based photocathode materials have come into the limelight as novel semiconducting materials for electron sources. However, due to the complexity of the growth process, they are still poorly characterized. Ab initio methods can contribute to fill this gap offering a tool to simulate them without the need for empirical parameters. In this work, we investigate K-Sb and Na-Sb binary crystals taking as an input structures available from computational databases. Adopting a high throughput workflow based on density functional theory, we evaluate the energetic stability of the scrutinized materials discarding unstable structures. For the remaining ones, we analyze the electronic properties focusing on the correlation between band-gaps and material composition. By calculating the band structure and atom-projected density of states, we gain further insights into the electronic properties of these systems. Our results provide an insight into the numerous intermediate phases that can form when growing alkali-based photocathodes and allow us to better understand the growth process.

MM 20.4 Tue 11:00 C 243

Predicting Equilibrium Pressure for Hydrogen Storage: A Cheminformatics Approach Using Deep Neural Networks — •Sinan S. Faouri[1,2], Kai Sellschopp[2], Paul Jerabek[2], and Claudio Pistidda[2] — [1]Applied Science private University — [2]Helmholtz-Zentrum hereon

Hydrogen storage is a critical aspect of hydrogen-based energy systems, and predicting the equilibrium pressure during storage processes is essential for optimizing storage conditions. In this study, we employ a cheminformatics approach by extracting a comprehensive set of descriptors, including electronegativity, electron affinity, atomic radius, thermal conductivity, and more, to characterize the hydrogen storage process. These descriptors serve as inputs for deep neural networks (DNNs) to predict the equilibrium pressure. We compare the performance of the DNN model against three other machine learning models to assess its predictive capabilities. The evaluation metrics of all four models are thoroughly examined and compared, providing insights into their respective strengths and weaknesses. This comparative analysis aims to elucidate the effectiveness of the cheminformatics-driven DNN approach in predicting equilibrium pressure for hydrogen storage, contributing to the advancement of efficient and reliable hydrogen storage technologies. The findings of this study have broader implications for the development and optimization of hydrogen-based energy systems.

MM 20.5 Tue 11:15 C 243

Peeling back the layers; Incorporating Dispersion Interactions and Quantum Mechanics at Clay Mineral Interfaces. — •Sam Shepherd, Gareth. A Tribello, and David. M Wilkins — Queen's University Belfast, Belfast, Northern Ireland, BT7 1NN

Clay minerals are complex layered materials whose unique structures allow them to be used in a range of processes. Accurately describing the interactions which take place between their layers however, remains a challenge. When studying these minerals theoretically, the need for accurate dispersion interactions is well understood, but accounting for the necessarily large system sizes and long timescales has hitherto limited theoretical study into these minerals.

To rectify this, we created a family of machine learned interatomic potentials (MLIPs), trained using dispersion corrected DFT calculations. We used these potentials to minimise computational expense while studying kaolinite for extended timescales. Thus, we have obtained structural and dynamical properties of kaolinite with previously unachievable levels of accuracy. Due to the nature of the interlayer interactions, we performed path integral molecular dynamics (PIMD) to include nuclear quantum effects (NQEs). This allowed us to perform simulations of kaolinite while treating the system fully quantum-mechanically.

We find that the addition of NQEs significantly impacts the dynamical properties of the system. This finding conclusively shows the need for full quantum mechanical approaches to gain a better appreciation of mechanistic processes like adsorption.

15 min. break

MM 20.6 Tue 11:45 C 243

Experiment-driven atomistic materials modeling: Combining XPS and MLPs to infer the structure of a-CO_x — •Tigany Zarrouk and Miguel Caro — Aalto University, Espoo, Finland

One facet of materials modelling is to gain insights from experimental results, which necessitates an effective strategy for identifying atomic structures that align with experimental data, *e.g.* spectra. Conventional approaches for amorphous materials involve generating numerous configurations through Molecular Dynamics and selecting one with the closest predicted spectrum to experiment. However, this process is inefficient and lacks assurance of spectrum conformity. We introduce a Grand-Canonical Monte Carlo methodology to generate configurations that concur with both experimental data and ab-initio calculations. Utilising a SOAP-based [1] X-Ray Photoelectron Spectroscopy (XPS) model trained on GW and Density Functional Theory (DFT) data, in conjunction with CO Gaussian Approximation Potential (GAP),

we identify oxygenated amorphous carbon structures compliant with experimental XPS predictions that are also energetically favourable within DFT. Clustering and embedding SOAP descriptors provides a data-driven deconvolution of the XPS spectrum into motif contributions, revealing the significant inaccuracies present in experimental XPS interpretation. This method generalises to multiple sets of experimental data and allows for the elucidation of specific experimental results, enhancing the applicability of materials modelling.
[1] Albert P. Bartók *et al.*: On representing chemical environments, Phys. Rev. B 87, 184115

MM 20.7 Tue 12:00 C 243

Exploring high-entropy alloy transport properties through the lens of machine learning — •Ruiwen Xie[1], Ye Wei[2], Bo Peng[3], Jiamu Liu[3], Liuliu Han[4], and Hongbin Zhang[1] — [1]Group of Theory of Magnetic Materials, Technical University of Darmstadt, Darmstadt, Germany — [2]École Polytechnique Fédérale de Lausanne (EPFL), Switzerland — [3]State Key Laboratory of Tribology in Advanced Equipment, Tsinghua University, Beijing, China — [4]Department Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung GmbH

The high-entropy alloys (HEAs), or the compositionally complexed alloys (CCAs), have attracted much attention due to their multifunctional properties with a vast chemical space to explore. For instance, the five-component HEAs contain approximately 4.6 million compositional combinations with a 1 at.% interval. Therefore, efficient sampling methods to navigate the chemical space for optimized properties are needed. As a showcase, we establish a workflow by combining the multi-objective Bayesian optimisation (MOBO) and active learning (AL), in order to explore the Ta-Nb-Hf-Zr-Ti system for compositions with optimal spin Hall conductivities and spin Hall angles. Additionally, a Monte Carlo beam search based AL algorithm is used to explore FeCoNi-based HEAs targeting for high saturation magnetization, high anomalous Hall conductivity and low electrical conductivity simultaneously.

MM 20.8 Tue 12:15 C 243

Machine-learning structural stability of complex intermetallic phases — •Mariano Forti, Ralf Drautz, and Thomas Hammerschmidt — ICAMS, Ruhr-Universität Bochum. Universitätsstr. 150 44801 Bochum

The understanding of the precipitation of topologically close packed (TCP) phases in single-crystal superalloys is of central importance for the design of these materials for high-temperature applications. However, the structural complexity of these intermetallic compounds and the chemical complexity of the superalloys with typically up to ten elements hampers the exhaustive sampling of chemical space by density-functional theory (DFT) calculations. For example, the computation of the convex hull of the R phase with 11 inequivalent lattice sites would require N^{11} DFT calculations in an N-component system. We overcome this computational limitation by combining machine learning (ML) techniques with descriptors of the local atomic environment of the TCP phases. In particlar, we use descriptors derived from bond order potentials (BOP) and atomic cluster expansions (ACE) that retain structural and electronic information. The resulting ML models predict the relative stability of complex TCP phases with very good precision in binary and ternary systems even for small training-data sets of only few hundred data points. We explore strategies for knowledge based feature selection that make it possible to handle the exponentially growing number of features in multicomponent systems, and to obtain a prediction for the convex hull of the R phase in Cr-Co-W system.

MM 20.9 Tue 12:30 C 243

Influence of the neighboring phases of MnS inclusions on damage accumulation in case-hardening steel — •Clara Reinhart[1], Tom Reclik[1], Maximilian A. Wollenweber[1], Ulrich Kerzel[2], Talal Al-Samman[1], and Sandra Korte-Kerzel[1] — [1]Institute for Physical Metallurgy and Materials Physics, RWTH Aachen University, Aachen, Germany — [2]Data Science and Artificial Intelligence in Materials and Geoscience, Faculty of Georesources and Materials Engineering, RWTH Aachen University, Aachen, Germany

Microstructural damage sites that are created during forming processes are usually observable in the form of voids and known to impede the mechanical properties of materials, especially during cyclic and rapid loading. In the case of 16MnCrS5 case-hardening steel, MnS inclusions lead to the creation of damage sites by cracking or delamination due to a pronounced mechanical contrast in the microstructure. This mechanical contrast depends on whether the inclusion is surrounded by ferrite, pearlite or both phases simultaneously. In this work we set out to characterize damage sites based on the neighboring phase of the MnS inclusion by training a machine learning network to automatically segment the etched microstructure and characterize the interfaces. In a second step damages sites are automatically detected and correlated to the determined neighboring phase(s). With this approach we show that a large difference of damage accumulation emerges for different neighboring phases, distinguishing not only inclusions with one-phase and two-phase interfaces, but also inclusions surrounded exclusively by either ferrite or pearlite.

MM 20.10 Tue 12:45 C 243

High-throughput damage quantification in steel and opportunities for damage-controlled forming processes — •Maximilian A. Wollenweber[1], Jannik Gerlach[2], Tom Reclik[1], Clara Reinhart[1], Sebastian Münstermann[2], Talal Al-Samman[1], and Sandra Korte-Kerzel[1] — [1]Institute for Physical Metallurgy and Materials Physics, RWTH Aachen University, Aachen, Germany — [2]Institute of Metal Forming, RWTH Aachen University, Aachen, Germany

When trying to improve the mechanical properties of steel parts a frequently overlooked cause for degradation of mechanical properties is the prevalence of damage sites often present in the form of voids in the microstructure. Caused by the mechanical contrast of different phases leading to plastic inhomogeneities during the forming process, these damage sites majorly decrease the longevity and crash performance. Trying to reduce these damage sites to enable damage-controlled forming processes poses two big challenges: On the one hand damage sites need to be characterized in order to understand the microstructural effects on damage formation and growth. On the other hand, optimized strain paths and adjusted microstructures need to be conceptualized to minimize the effect of damage on the performance. In this work we want to exemplary show how to tackle both of these issues; how high-throughput scanning electron microscopy and artificial intelligence can be used to evaluate damage sites, as well as demonstrating how adjustments to the strain-path and different microstructural concepts harbor opportunities for damage-controlled forming processes.