

MM 27: Data Driven Material Science: Big Data and Workflows IV

Time: Tuesday 14:00–14:45

Location: C 243

MM 27.1 Tue 14:00 C 243

A comprehensive screening of plasma-facing materials for nuclear fusion — ●ANDREA FEDRIGUCCI¹, PAOLO RICCI¹, and NICOLA MARZARI^{1,2} — ¹École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — ²Paul Scherrer Institute, Villigen, Switzerland

Plasma-facing materials (PFMs) represent one of the most significant challenges for the design of future nuclear fusion reactors. Inside the reactor, the divertor experiences the harshest material environment: intense bombardment of neutrons and plasma particles coupled with extremely large and fluctuating heat fluxes. The material chosen to cover this role in the fusion reactor ITER is tungsten. While no other material has shown the potential to match the properties of W, many drawbacks associated with its application remain. This work aims to produce a structured and comprehensive materials screening of candidate PFMs based on known crystal structures. The methodology to identify the most promising PFMs combines peer-reviewed data of inorganic crystals from the Pauling File database and first-principles DFT calculations of two key PFMs properties, namely the surface binding energy and the formation energy of a hydrogen interstitial. The materials that meet the necessary thermal performance to withstand heat loads are critically compared with the state-of-the-art literature, defining an optimal subset where to perform first-principles calculations. The majority of well-known PFMs - such as W, Mo, and carbon-based materials - are captured by this screening process, along with less familiar refractory materials that warrant further investigation.

MM 27.2 Tue 14:15 C 243

Machine learning modelling of local magnetic moments in Fe-based intermetallic compounds — ●BO ZHAO¹, KUN HU², and HONGBIN ZHANG¹ — ¹Institute of Materials Science, Technische Universität Darmstadt, Peter-Grünberg-Str. 2, 64287 Darmstadt, Germany — ²School of Materials Science and Engineering, Central South University, Changsha, 410083, Hunan, PR China

It is well known that the magnitude of magnetic moments is determined by the local crystalline environments as verified by studying the dimensional crossover behavior of a few representative systems such as Fe. To further generalise and quantify the mapping between the crystal environments and magnetic moments, we carried out machine learning

modelling on Fe-based intermetallic compounds, with the corresponding magnitude of magnetic moments for Fe atoms varying between zero and four Bohr magneton (the atomic limit). Using the symmetry-adapted smooth overlap of atomic positions (SOAPs) as descriptors, it is observed that 2374 data for binary and ternary compounds collected from Materials Project are not sufficient for a reliable modelling. We further enriched the dataset by performing high-throughput calculations on Fe-(B, Co, Ti, Rh) binary intermetallic compounds, and the corresponding accuracy of the machine learning modelling is over 90% across all the systems. The results are further understood based on the Stoner model. Our work establishes a valid approach to model the physical properties dependent on the local crystalline environments.

MM 27.3 Tue 14:30 C 243

Synergistic catalytic sites in high-entropy metal hydroxide organic framework — ARKENDU ROY, ●SOURABH KUMAR, ANA GUILHERME BUZANICH, TILMANN HICKEL, FRANZISKA EMMERLING, and BISWAJIT BHATTACHARY — BAM, Bundesanstalt für Materialforschung und -prüfung, Richard-Willstätter-Str. 11, 12489 Berlin

Leveraging data-driven computational techniques accelerates catalytic process analysis and prediction, enabling materials discovery and chemical reaction optimization. Among such materials, high-entropy metal hydroxide organic frameworks (HE-MHOFs), with intricate structures surpassing conventional MOFs, are of special interest. In HE-MHOFs, high-entropy hydroxide layers are connected by ligands to form a superlattice, introducing structural disorder and diversity. Using the state-of-art ab initio calculations, the HE-MHOFs have been designed based on the stability of unary MHMOFs by constructing their ab initio Pourbaix diagram, followed by their synthesis using a conventional solvothermal process. The incorporation of different transition metals (TMs) alters the electronic structure, influencing adsorbate binding energy and catalytic activation potential. The SQS approach is used to deconvolute the atomic patterns and sample out the most favourable surfaces for OER investigations. Then the complexities in the proton-coupled electron transfer OER reaction mechanism are addressed by constructing a potential energy surface for each redox-active TM and comparing it to parent unary MOFs. A confirmation through in-situ XPS and EDX mapping complements our computational approach.