Modelling Hydrogen–Transition Metal Interactions on Carbon Platforms with Universal ML Interatomic Potentials

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Carbon-based nanoporous and layered materials doped with transition metals (TM) are promising candidates for hydrogen storage platforms according to Density Functional Theory (DFT) studies [1,2]. However, modelling the adsorption/desorption of hydrogen under realistic conditions requires large-scale Ab Initio Molecular Dynamics (AIMD) simulations that are computationally prohibitive. In this context, universal Machine Learning Interatomic Potentials (uMLIPs) provide transferable and computationally efficient models capable of capturing DFT accuracy across large systems and long timescales [3].

In this work, we tested different uMLIPs on TM–carbon platforms. In particular, we examined its performance on properties such as thermal stability, radial distribution function, adsorption energies and geometries of TM atoms/clusters, diffusion pathways and migration barriers, and vibrational properties. Our results showed that MACE-MH_OC20 and NequIP-OAM-XL models, despite not being specifically trained on our target TM-carbon platforms, agree with the main structural, energetic, and dynamical properties observed in DFT. Then, we fine-tuned both uMLIPs models using a large and diverse dataset that includes a wide range of TM clusters and carbon-based layers (including defective ones), mostly generated from AIMD simulations covering near- and out-of-equilibrium structures. Our aim is to train a model that can be reliably transferred for dynamic catalytic studies. Finally, extensive MD simulations of hydrogen adsorption and desorption will be performed to evaluate the hydrogen storage capacity of TM-carbon platforms under practical conditions.

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