Contribution ID : **134** Type : **Poster Presentation**

Towards a Generalizable Machine Learning Potential for Water Adsorption within MOFs

Direct air capture (DAC) is a promising strategy to mitigate atmospheric CO_2 concentrations, requiring adsorbents with high CO_2 affinity and low water affinity. Metal–organic frameworks (MOFs) are attractive candidates for DAC due to their structural tunability and high porosity.

While high-throughput computational screening studies have been conducted to find the optimal MOFs1, accurately predicting water adsorption enthalpy remains challenging, as classical force fields often fail to capture hydrogen bonding and typically assume a rigid framework. These limitations can be addressed using machine learning potentials (MLPs) trained on flexible MOF structures with one adsorbed H_2O. For example, in CAU-10 with one H_2O molecule per unit cell, the water adsorption enthalpy predicted by the universal force field (UFF) is 26 kJ/mol, which is significantly lower than the experimental value of 52 kJ/mol. In contrast, the MLP predicts 44.5 kJ/mol, which is in much better agreement with experiment.

We develop a data-efficient approach to train a generalizable MLP for Al-MOFs, achieving energy errors below 1 meV/atom and force errors below 30 meV/Å, with fewer than 400 configurations required per MOF. Validation against experimental data for five Al-MOFs confirms the accuracy of our method, enabling DFT-level predictions of water adsorption enthalpy for DAC screening.

Primary author(s) : Mr. LI, Yutao (EPFL)

Co-author(s) : Mr. ZHANG, Xiaoqi (EPFL); Mr. JIN, Xin (EPFL); Prof. SMIT, Berend (EPFL)

Presenter(s) : Mr. LI, Yutao (EPFL)