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Predicting Adsorption Energies for Methanol Electro-oxidation Intermediates on Pt: A Machine Learning Approach

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The accurate determination of the adsorption energy (E_{Ads}) for the methanol electro-oxidation reaction (MEOR) intermediates over platinum is an important contribution to the development of more efficient catalysts [1]. Computational methods are a powerful tool to determine this parameter, which is still dependent on highly time consuming methods for an accurate determination. In this study, the equiformer_v2 model, which was pre-trained on E_{Ads}, was utilized to predict the E_{Ads} of a group of possible alcohol electro-oxidation intermediates with known experimental E_{Ads} values and similar bonding features on Pt as the intermediates of the MEOR. The Atomic Simulation Environment package was utilized to perform the energy calculations and build the Pt slabs. The difference between the calculated EAds and the experimental values, obtained on the ADS41 database [2], are shown in Fig. 1.

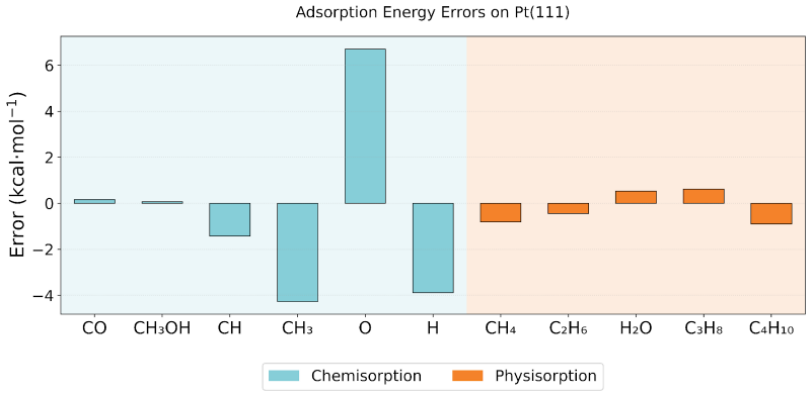

Fig. 1 - Experimental and ML obtained adsorption energy difference over Pt(111).

For the physisorbed systems, the errors are, overall, smaller than the chemisorbed ones, except for CO and CH3OH. The errors are similar to the ones Araújo et al. [3] obtained with PBE+D3, but the calculations are much faster than a density functional theory calculation. However, the model, for some cases, is still far from the chemical accuracy. Thus, the equiformer_v2 model will be fine tuned within the Fairchem module and with electronic structure calculations, performed on the Orca 6 program package, which will both help improve the accuracy for the above adsorbates and for the intermediates of the MEOR.

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