Density Functional Theory Insights into Electro-Hydrogenation of Furfural on CoxMoOy-Decorated Activated Carbon Catalysts

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Abstract:
The electrochemical hydrogenation (ECH) of biomass-derived furfural (FF) into valuable chemicals, such as furfuryl alcohol (FA) and tetrahydrofurfuryl alcohol (THFA), is a promising pathway for sustainable chemical and fuel production. However, large-scale ECH applications are limited by the complexity of reaction mechanisms and a lack of understanding regarding optimal catalytic parameters. This study employs density functional theory (DFT) to investigate the reaction mechanisms and energetics of FF electro-hydrogenation on activated carbon (AC) electrodes enhanced with CoxMoOy catalysts. These catalysts, including MoO2, MoO3, and MoCoO4, were selected based on their electrochemical potential for improved wettability and FF adsorption on AC surfaces. Activated carbon was chosen for its high surface area, tunable porosity, and role as a sustainable electrode support derived from biomass processing byproducts like bio-char [1]. Using the Vienna Ab initio Simulation Package (VASP), DFT calculations assessed the adsorption energy of FF with and without solvation across the four catalyst configurations (pure AC, MoO2/AC, MoO3/AC, and MoCoO4/AC) [2]. MoCoO4/AC exhibited the highest adsorption energy for FF, attributed to the unique interaction facilitated by cobalt's addition, which enhances both wettability and electron transfer efficiency on the electrode surface. This configuration offers an energetically favorable pathway for FF conversion, with implications for optimizing faradic efficiency and selectivity toward FA production [3]. The DFT results suggest that MoCoO4 on AC improves FF conversion efficiency by maximizing electron transfer and creating a surface conducive to reactant adsorption. The strong affinity of MoCoO4 for FF, combined with favorable reaction pathways, highlights its potential for scalable electrocatalyst applications. These findings offer a predictive framework for designing efficient electro-catalysts in sustainable biomass valorization, presenting a pathway for bio-based chemical materials that can be used as raw material for sustainable fuel production as FF can further be hydrogenated to fuel formulations. Further investigations, including nudge elastic band (NEB) calculations, were performed to explore selectivity and yield optimization, aiming to bridge laboratory findings with industrial feasibility.

References

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Figures

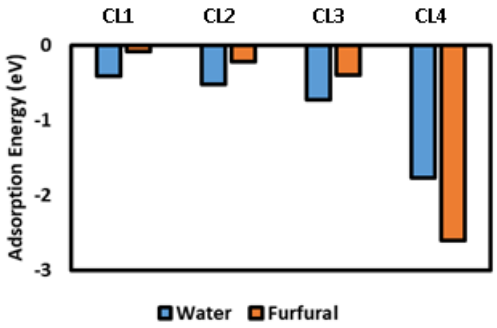

Figure 1: Adsorption energies of water (H_2O) and furfural (FF) on various electrode surfaces: carbon layer (CL1), AC layer with MoO_2 (CL2), AC layer with MoO_3 (CL3), and AC layer with $MoCoO_4$ (CL4).