

A Molecular Dynamics Study of Myo-Inositol at Platinum-Water interface

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Abstract

Alkaline Hydrogen Evolution Reaction (HER) on a Pt electrode is limited by its sluggish kinetics but shown to have benefits over acidic HER due to its cost effectiveness. In previous experiments, small organic molecules such as caffeine have shown to improve alkaline HER significantly due to the ability to change interfacial hydrogen bonding networks. Inspired by this approach, we explored the application of Myo-inositol (MI) which is known to influence hydrogen bonding structure of water. MI show improvement in Alkaline HER¹. Interestingly, other carbohydrates do not cause comparable enhancement of the reaction. To understand the mechanism of action, I employed molecular dynamics (MD) simulations of MI solution in the presence of Pt surface.

The simulations used Pt surface and water solution of ~1 molar MI and four negative controls: galactose, glucose, mannitol and sorbitol. We generated 1 μ s simulations to record interfacial density profile, contact-state, hydrogen bonding network, and second layer dynamics to access molecular population density, hydrogen bonding disruption, water/sugar accessibility to Pt surface, and sugar survival across various layers.

The results of the analysis showed a significant difference in interfacial water retention of the MI-Pt system relative to the other sugar-Pt system. Contact state and density profile analysis showed that the MI-Pt system left significantly more water accessible to Pt compared to the other sugars. Within the direct interfacial surface layer, MI preserves the highest water density among the other sugar systems, maintaining water-water hydrogen bonding, and exhibits larger and more persistent second interfacial layer sugar population.

Together, we hypothesize that the more effective alkaline HER results from dynamic adsorption of MI on a Pt surface which reorganize the water-water hydrogen bonding network at the interface between the electrode and water while also allowing for significant electrode access. This contrasts with other sugars, which show stronger adsorption on the Pt and decrease the water exchange.

References:

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