First-principles molecular dynamics (FPMD) simulations of Co_3O_4/acqueous solutions interfaces: electrocatalysis & water splitting

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The processes involved in electrochemistry at the solid-liquid-electrolytic interface in order to produce molecular hydrogen and oxygen is a current key field of research in science and technology, especially of importance for the hydrogen economy, for green technology in a period of time with an ever more growing demand in green-energy. In this context, water splitting at cobalt oxide interfaces has to be investigated in details, and molecular simulations are highly relevant in order to understand the mechanisms at play, how the oxides can act as a good catalyst for the water splitting, and how liquid water at the interface can be involved in the overall processes. Most of the existing first-principles calculations published in the literature on Co_3O_4 oxides are related to "surface science" calculations[1-4], where there is no explicit introduction of interfacial water molecules.

We report on DFT-based molecular dynamics simulations of the (110) Co_3O_4-liquid water interface, in electrocatalysis conditions. We will present our modeling of this complex inhomogeneous interface and its characterization in terms of interfacial structure (solid surface and interfacial water), dynamics and chemical reactivity (e.g. adsorption and dissociation of interfacial water, transfers of protons, H-bond environments, speciation, orientation of surface hydroxyls, effect of electric field, etc.).

References

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