First-Principles Prediction of the Electrochemical Stability of Bimetallic Catalysts for Use as Fuel Cell Electrodes

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Fuel cells are electrochemical devices that convert the energy of a fuel into electricity using a catalyst such as platinum or palladium. These catalysts are, however, scarce and pricy, which is imposing serious constraints on the massive deployment of fuel cell electric vehicles. By alloying the catalyst with a cheaper metal, it is possible to alleviate these constraints without reducing the conversion efficiency of the electrode. It is even feasible, in some instances, to improve the activity of the alloy beyond that of the pure catalyst; this type of improvement is observed when the chemical (ligand) or physical (strain) effects that arise from alloying bring the catalyst closer to the top of the volcano plot that relates the catalytic activity of the electrode to the energy of the adsorbed oxygen and hydrogen species. This presentation will discuss recent progress in the quantum–continuum multiscale modeling of solid–solution interfaces [1-4] using the QUANTUM-ESPRESSO software [5-6] to accelerate the development of bimetallic catalysis with a focus on answering the critical question of their surface stability under the operating conditions that are relevant to fuel cell systems.

References

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