DFT study of polymers coated palladium nanoparticles for H_2 sensing

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Palladium-based materials have been known for long for their capacity to form hydride phases, making them good candidates for hydrogen storage applications. They can also be used to form hydrogen-selective membranes, for example useful for separation and purification of hydrogen[1], or for hydrogen sensing. These applications rely on two fundamental features of metallic palladium: the ability to dissolve hydrogen to form stable hydride and the possibility to easily release the stored hydrogen.

Efforts have been made to improve the storage capacity and kinetics, either by modification of the metallic core (alloys or core-shell structures) or by varying the environment of the palladium material. Experimentally, the presence of metal-organic frameworks[2] or polymers[3,4] has been shown to improve the kinetics of hydrogen storage.

Using DFT, we try to shed light on how this phenomenon can be explained. We propose a large scope model for this system, going from the modelling of H_2 diffusion in a polymer matrix to the study of subsurface hydrogen diffusion in palladium hydride *via* the comprehension of the processes occuring at the polymer-metal interface.

In order to do this, the stability of palladium hydride nanoparticles is studied, and the effect of several polymers (PTFE, PVDF and PMMA) coating on H_2 adsorption/desorption as well as subsurface diffusion is considered. Rationalization on how and why the polymers affect the metal NP is proposed. The diffusion of H_2 molecules in polymer environment is studied as to take into account a realistic medium for those nanoparticles. Finally, the challenging task of properly describing the metal NP – polymer interface is adressed in order to be able to give an as complete and as accurate as possible view of the whole phenomenon.

[1] Renewable Sustainable Energy Rev. 2015, 47, 540.
[2] Nature Materials, 2014, 13, 802-806
[3] ChemCatChem 2016, 8, 1646 – 1650
[4] Angew. Chem. Int. Ed. 2014, 53, 12081 –12085