Title: **Fate of Hydrogen on fcc Metals**
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Date: June 2019
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Transition metals with a face-centered cubic *(fcc)* arrangement are prone to be used as catalysts in heterogeneous catalysis. Their ability to capture hydrogen makes them an interesting object of study given the importance of hydrogenation reactions in the chemical industry. This study simulates by means of a computational study the stability of the hydrogen in the surfaces of the *fcc* transition metals for different packing arrangements, which are (001), (011) and (111).

The study is carried out by the density functional theory (DFT), which using exchange and correlation functionals is intended to find the values of adsorption and absorption energies to evaluate the predisposition of metals to form an optimal surface-substrate association for future applications in heterogeneous catalysis. The minimal energy will be found for different positions on the surface and subsurface, evaluating whether the metal has a preference for hydride formation, hydrogen adsorption or if it is preferred not to incorporate hydrogen and keep it in molecular form.

As expected, the results showed that noble metals tend to reject the adsorption and absorption of hydrogen, because they are more stable alone. There is a general predisposition in all the transition metals studied for preferring adsorption instead of absorption except for Palladium, that although preferring adsorption, whose affinity for both reactions is competitive.

Keywords: Density functional theory, correlation and exchange, heterogeneous catalysis, transition metals, fcc, hydrogenation, adsorption, absorption.

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