Title: **Hydrogen adsorption and absorption on hcp metals**
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Transition Metals (*TMs*) are materials in widespread use in industry and technology. Their use in hydrogenation processes is a main field. There, atomistic information of the interaction of H on TM surfaces, or its incorporation, is key for future development on the diverse research fields. This information is accessible through Density Functional Theory (*DFT*) simulations, especially to gain trends along and across the Periodic Table. Here, those TMs with a hexagonal close-packed (*hcp*) crystallographic structure are studied as they are useful targets, being spread along the Periodic Table, enabling the sought trend capturing. The H adsorption or absorption is analyzed based on accurate DFT simulations, on realistic surface slab models, exploring the most-stable (0001), ($10\bar{1}0$), ($11\bar{2}0$), *hcp* TM surfaces.

The results show a clear preference for adsorption, thus reveling that the hydride formation in thermodynamically inhibited at low coverages. Aside, a clear trend is observed, as the larger the number of *d* electrons, the, weaker the H bonding. However, although the *d*-band center model captures this trend, the values cannot be used as a quantitative chemical descriptor, pointing out that other factors —surface energies, surface saturation— which can be determining to the bonding strength.

Keywords: *hcp* transition metals, heterogeneous catalysis, density functional theory, adsorption, absorption, hydrogen atom.