Abstract Submitted
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The chemical potential of hydrogen in Mg-films and metal-doped carbon nanostructures[1] MINA YOON, Oak Ridge National Laboratory and Fritz-Haber-Institut der Max-Planck-Gesellschaft, HANNO WEITERING, ZHENYU ZHANG, Oak Ridge National Laboratory — We use first-principles density functional theory to study the binding mechanism of hydrogen to nanoscale systems. We investigate the performance of the exchange-correlation functional in describing the interaction between hydrogen and metal systems and the importance of the vibrational contribution in the formation enthalpy. In ultrathin Mg films the stability of hydrides is much lower than in the corresponding bulk systems and it can be modified by metal alloying. We calculate the chemical potential of hydrogen in Mg films for different dopant species and film thicknesses while including all vibrational degrees of freedom. By comparing the chemical potential with that of free hydrogen gas at finite temperature and pressure, we construct a hydrogenation phase diagram and identify the conditions for hydrogen absorption/desorption. The vibrational contribution to the chemical potential of hydrogen becomes more prominent for dihydrogen adsorption to metals, where its significance dramatically changes depending on the binding characteristics. This feature is illustrated by the example of metal-doped nanocarbon systems.

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