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Title: Nanoscale metal hydrides for hydrogen storage: effects of size and composition

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In an effort to further extend the search for high quality hydrogen storage materials, we used the very accurate electronic quantum Monte Carlo simulations to calculate the hydrogen desorption energy of nanoscale metal hydrides. At sizes around 1 nm, our calculations predict that Al/Mg alloyed nanoparticles are stable and the metal composition can be tuned to tune the hydrogen absorption energy, enabling the material to be charged and discharged reversibly. We also compare to lower level methods such as density functional theory, which are qualitatively, not quantitatively accurate for the calculation of the enthalpy of absorption of H$_2$.