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Calcium-Decorated Carbon Nanotubes for Hydrogen Storage[1]
HOONKYUNG LEE, University of California Berkeley, JISOON IHM, Seoul National University, MARVIN L. COHEN, STEVEN G. LOUIE, University of California Berkeley — Using the first-principles pseudopotential density-functional method, we carry out a systematic search for high-capacity hydrogen storage media based on individually dispersed calcium atoms on carbon nanotubes (CNTs). We find that Ca clustering is suppressed on boron-doped and defective carbon nanotubes and that up to six H_2 molecules can bind to a Ca atom with a binding energy of $\sim$0.2 eV/H_2. We show that Ca-decorated CNTs with a concentration of $\sim$6 at. % B doping can reach the gravimetric capacity of $\sim$5 wt % hydrogen storage. We also will discuss the binding mechanism of the H_2 molecules.

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