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Quantum Monte Carlo studies of the non-dissociative absorption of hydrogen to doped fullerenes ANDREW WILLIAMSON, Lawrence Livermore National Laboratory, YONG-HYUN KIM, SHENGBAI ZHANG, National Renewable Energy Laboratory — The reversible storage of hydrogen at room temperature requires an adsorption energy in the range of 0.2 to 0.6 eV per hydrogen molecule. However, there are currently no storage materials which have been shown to bind hydrogen with this energy. Typically, hydrogen either retains its molecular form, and binds only weakly via a van der Waals interaction, or it dissociates into atoms and forms strong covalent bonds. Here we present the results of first-principles density functional and Quantum Monte Carlo calculations of the non-dissociative absorption of hydrogen molecules to doped carbon fullerenes. These calculations reveal significantly enhanced binding of hydrogen to substitutional B and Be doped fullerenes. Our Quantum Monte Carlo and benchmark quantum chemistry calculations are used to evaluate the accuracy of different exchange correlation functionals for describing the hydrogen adsorption interaction. We find that the LDA functional significantly overestimates the binding energy of hydrogen, while GGA functionals underestimate the binding energy. This work was performed under the auspices of the US Department of Energy by the University of California, Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48

Andrew Williamson
LLNL

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