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Predicted high storage of hydrogen via H2 complexes on titanium-decorated nanotubes TANER YILDIRIM, National Institute of Standards and Technology, Gaithersburg, MD 20899, USA, S. CIRACI, Physics Department, Bilkent Univeristy, Ankara, Turkey — Developing safe, cost-effective, and practical means of storing hydrogen is crucial for the advancement of hydrogen and fuel- cell technologies. The current state-of-the-art is at an impasse in providing any materials that meet a storage capacity of 6wt% or more required for practical applications. Accurate quantum mechanical calculations that predict new materials or routes to engineering materials properties are important to overcome this barrier. Here we report a first-principles study, which demonstrates that a single Ti atom coated on a single-walled nanotube (SWNT) strongly binds up to four hydrogen molecules. The first H2 adsorption is dissociative with no energy barrier while other three adsorptions are molecular with significantly elongated H-H bonds. At high Ti coverage we show that a (8,0) SWNT can strongly adsorb up to 8wt% hydrogen. Simulations at high temperature indicate that the system is quite stable and exhibits associative desorption upon heating, a requirement for reversible storage. These results not only advance our fundamental understanding of dissociative adsorption of hydrogen on transition metals in nano-structures but also suggest new routes to better storage and catalyst materials.

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