

Abstract Submitted
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On the Hydrogen Storage Capacity Limitations of Carbon Nanotube Bundles DIMITRIOS MAROUDAS, ANDRE MUNIZ, University of Massachusetts Amherst — Exposure of single-walled carbon nanotubes (SWCNTs) to atomic hydrogen leads to chemisorption of H atoms on the SWCNT walls, enabling the use of SWCNTs as hydrogen storage media with a theoretical storage capacity of 7.7 wt%. Experimental studies, however, have reported inconsistent hydrogen storage capacities that are usually well below this limit. To explain the experimental measurements, we have developed an analytical model that describes the effect of SWCNT swelling upon hydrogenation on the hydrogen storage capacity of SWCNT bundles. The model is properly parameterized using a large set of atomistic simulation results for the dependence of SWCNT swelling on the degree of hydrogenation as measured by the coverage of the SWCNTs by chemisorbed atomic H. The model generates experimentally testable hypotheses, which can be used to explain the lower H storage capacities reported for SWCNT bundles and the experimentally observed nonuniform hydrogenation of SWCNT bundles. It also provides recommendations for optimal SWCNT arrangement in bundles to maximize their hydrogen storage capacity.

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