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Hydrogen inside fullerene nanocage OLGA PUPYSHEVA, AMIR FARAJIAN, BORIS YAKOBSON, Rice University, Houston, TX 77005 — We model fullerene nanocages filled with hydrogen using density functional theory. Stability of such endohedral complexes is studied depending on the amount of encapsulated hydrogen. It is shown that some of the hydrogen atoms can be chemisorbed on the inner surface of the nanocage. The mechanism of cage breaking is investigated by ab initio molecular dynamics simulations, and the hydrogen chemisorption, which weakens the fullerene C-C bonds, is proved to play the key role in this process. We also discuss the mechanical properties of fullerene nanocage and find the internal hydrogen pressure on the nanocage.

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