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The design of a nanocontainer for high pressure storage of hydrogen[1] ZHI-FENG LIU, Chinese University of Hong Kong, DEYAN SUN, East China Normal University, XIANG YE, XINGAO GONG, Fudan University
— Molecule hydrogen is known to have a weak van der Waals potential, which makes it difficult to raise its storage efficiency for physisorption based methods. In this report, we explore the other side of such a weak potential, the well-known compressibility of hydrogen. A (20,0) single wall carbon nanotube based nanocontainer is designed, in which a C_{60} "peapod" at the cap section of the nanotube serves as a molecular valve. Diffusion barriers through such a valve is examined by molecular dynamics simulations under various conditions. It is demonstrated that H_2 can first be filled into the container upon compression at low temperature, and then be locked inside it after the release of external pressure. The internal pressure that can be achieved in this design is in the GPa range at room temperature, which is much higher than the typical pressure of a few hundred bar currently employed for hydrogen storage. At 2.5 GPa, the storage weight ratio approaches a promising 7.7%.

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