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Density Functional Calculation of Hydrogen Storage in a C_{60} Molecule[1] CHIH-KAI YANG, Chang Gung University — Storage of hydrogen molecules is a research topic that has deep scientific interests and enormous applications in providing a clean type of energy for the future. Recent experimental breakthrough in encapsulating hydrogen molecules in fullerene C_{60} promises a wider role for the versatile carbon cage in this regard. Probing further, we use density functional theory to study how the enclosed hydrogen molecules interact with the carbon cage. The calculations show that quite a few molecules can be exothermically inserted into the cage and as many as 35 hydrogen molecules can be stored inside without rupturing the cage structure.

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