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**Study on Ca32C60 Cluster for Hydrogen Storage**[1] PING CUI, ZHILING DUN, MENG YE, RAN TAO, HAIPING LAN, U of Science and Technology of China, ZHENYU ZHANG, Oak Ridge National Laboratory, U of Tennessee-Knoxville, U of Science and Technology of China — Using first-principles calculations within density functional theory (DFT), we study the assembly of Ca32C60, the most desirable metal-coating fullerene as hydrogen storage medium. We first explore possible structures of Ca32C60 dimer with different initial configurations, and find a surprisingly large binding energy up to 2.8 eV. Our further analysis on electronic structures indicates that such a large binding strength stems from the enhanced chemical reactivity of Ca due to the Ca-3s valence electrons partially transferred to the fullerene. We then systematically investigate the alkali and alkali earth elements coated on fullerene, and find that the chemical reactivity of these metal elements can be tuned due to the large electron affinity of C60. Based on this finding, we then extend our studies to the bulk form and two-dimensional structures of Ca32C60, and propose an optimum assemble structure for hydrogen storage. These results shall facilitate designing and optimizing carbon-based materials for hydrogen storage.

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