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Theoretical study of hydrogen storage in Ca-coated fullerenes QIANG SUN, Peking University and Virginia Commonwealth University, QIAN WANG, Virginia Commonwealth University, YOSHI KAWAZOE, Tohoku University, PURU JENA, Virginia Commonwealth University — First principles calculations based on gradient corrected density functional theory and molecular dynamics simulations of Ca decorated fullerene yield some novel results: (1) C60 fullerene decorated with 32 Ca atoms on each of its 20 hexagonal and 12 pentagonal faces is extremely stable. Unlike transition metal atoms that tend to cluster on a fullerene surface, Ca atoms remain isolated even at high temperatures. (2) C60Ca32 can absorb up to 62 H2 molecules in two layers. The first 30 H2 molecules dissociate and bind atomically on the 60 triangular faces of the fullerene with an average binding energy of 0.45 eV/H, while the remaining 32 H2 molecules bind on the second layer quasi-molecularly with an average binding energy of 0.11 eV/H2. These binding energies are ideal for Ca coated C60 to operate as a hydrogen storage material at near ambient temperatures with fast kinetics. (3) The gravimetric density of this hydrogen storage material can reach 5.8 wt %. Simple model calculations show that this density is the limiting value for higher fullerenes.

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