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Light Alkaline-Earth-Metal Coated Carbon Fullerenes as Effective Hydrogen Storage Media[1] MINA YOON, ORNL/U. of Tennessee, SHENYUAN YANG, Chinese Academy of Sciences/U. of Tennessee, CHRISTIAN HICKE, Michigan State U., ENGE WANG, Chinese Academy of Sciences, DAVID GEOHEGAN, ORNL, ZHENYU ZHANG, ORNL/U. of Tennessee — We propose functionalizing carbon nanostructures with light alkaline-earth metals for use as hydrogen storage media. To support this idea, we investigate the feasibility of coating C_{60} fullerenes with light alkaline-earth metals and analyze the hydrogen storage capacities of the resulting compounds. We find a new and unique binding mechanism responsible for the strong binding between Ca or Sr atoms and C_{60}. Our theory explains experiments showing that C_{60} can be evenly covered by a monolayer of Ca or Sr atoms. The coating results in a charge redistribution leading to electric dipolar fields around the metal atoms through which the fullerene surface becomes an ideal hydrogen-attractor with a binding strength larger than that of alkali carbon complexes but small enough to prevent hydrogen dissociation as in the case of transition metal decorated fullerenes. With a hydrogen uptake of more than 8.4wt% and a binding energy of $\approx$ 0.4eV/H2 on $C_{60}C_{32}$ Ca is superior to currently used coating elements.

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