Hydrogen storage on calcium coated boron (hetero-)fullerenes: A DFT study

SULEYMAN ER, Harvard University, GEERT BROCKS, University of Twente, GILLES A. DE WIJS, Radboud University Nijmegen — Using density functional theory (DFT), we investigate hydrogen storage properties of calcium-coated molecular systems of B$_{80}$ boron fullerene, C$_{48}$B$_{12}$ boron-doped heterofullerenes, and well-known C$_{60}$ fullerene. Here, we consider the most common and low-lying isomers of B$_{80}$ and C$_{48}$B$_{12}$. We find that the Ca-coated molecules have the following properties: (1) The binding of metal atoms to B$_{80}$ or to C$_{48}$B$_{12}$ molecules is much stronger than their binding to a C$_{60}$ molecule. (2) B$_{80}$ and C$_{48}$B$_{12}$ have larger electron affinities than their carbon only counterpart, and accordingly discharge the surface Ca atoms more efficiently. (3) B$_{80}$ molecule, however, shows structural deformations upon reacting with Ca atoms. (4) C$_{48}$B$_{12}$Ca$_{6}$, however, is stable at elevated temperatures. C$_{48}$B$_{12}$ has well-exposed, positively charged Ca atoms on its surface, and binds up to six hydrogen molecules per metal center with hydrogen binding energies of 0.17-0.14 eV/H$_2$, that are suitable for ambient temperature hydrogen storage.

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