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Ca coated boron nanostructures: Energetics and possible usage for hydrogen storage TUNNA BARUAH, MARCO OLGUIN, RAJENDRA ZOPE, University of Texas at El Paso — We investigate the adsorption of calcium atoms on the surface of novel boron fullerenes and the alpha boron sheet using density functional theory within the generalized gradient approximation. Recent theoretical works show that the B_{80} fullerene coated with one Ca atom on each pentagonal ring is capable of storing up to 60 H_2 molecules, yielding a gravimetric density of 8.2 wt.%. We have performed a detailed investigation of Ca adsorption on the B_{80} fullerene. In contrast to recent results, our calculations show that a single Ca atom prefers to occupy a hexagonal site rather than a pentagonal site. The calculations on $Ca_{12}B_{80}$, $Ca_{20}B_{80}$ and $Ca_{32}B_{80}$ indicate that Ca atoms prefer to uniformly coat the whole surface over selectively occupying the pentagonal or hexagonal sites. We have examined the feasibility of H_2 storage on $Ca_{32}H_{80}$ in the range 7.2 - 8.2 wt%. Our calculations indicate that the uniformly coated $Ca_{32}B_{80}$ fullerene is not capable of achieving a hydrogen storage capacity of 7.2 wt. % or higher. It is necessary to somehow reduce the Ca concentration on the B_{80} surface to achieve a 8.2 wt. % of hydrogen.

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