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Hexagonal Antiprismatic Metallacarborane Clusters for Hydrogen Storage CÜNEYT BERKDEMIR, PING LIN, JORGE SOFO, Penn State — We investigated the adsorption properties of molecular hydrogen attached to hexagonal antiprismatic metallacarborane clusters, $RuNiC_2B_{10}H_{12}$ and $Ru_2C_2B_{10}H_{12}$, using density functional theory. These clusters have been recently synthesized using the reduction-metallation (RedMet) approach [1] and their structures have been resolved. The hydrogen molecules are sequentially attached to these clusters until the H_2 binding energies fall below 0.2 eV, which is the minimum value of ideal H_2 binding energy in the range of 0.2-0.4 eV/H_2 for the practical vehicle applications [2]. We included the van der Waals interactions between metallacarborane clusters and molecular hydrogens. We also evaluated the contribution of zero point vibrational energies to the H_2 binding energy. The kinetic stability of these clusters before and after hydrogen adsorption is discussed by analyzing the energy gap. The results show that $RuNiC_2B_{10}H_{12}$ and $Ru_2C_2B_{10}H_{12}$ clusters can bind up to 8.5 wt % and 9.8 wt % molecular hydrogen, respectively. These results suggest that these metallacarborane clusters are potential hydrogen storage materials to meet the targets of DOE for 2015.

[1] D. Ellis et al., Chem. Commu. **14**, 1917 (2005).
[2] http://www.sc.doe.gov/bes/hydrogen.pdf.

Jorge Sofo
Penn State

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