"Supporting Information"

Metal decorated carbon-doped BN fullerenes as highly efficient materials to solid-state hydrogen storage: Insights from DFT calculations

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Figure S1. Optimized geometries of different C-doped BN nanostructures considered in the present study

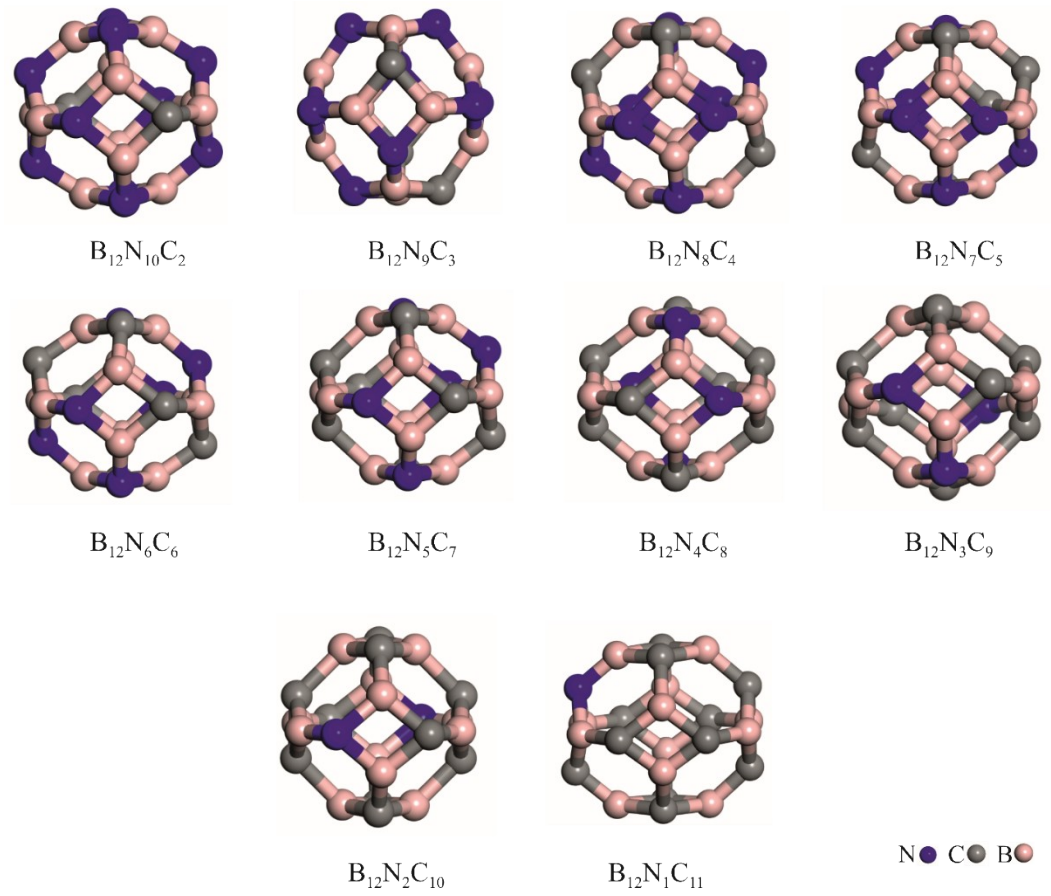

Figure S2. Optimized geometry and adsorption energy of a Li (left) or Sc atom (right) adsorbed on the pure $B_{12}N_{12}$ nanocage

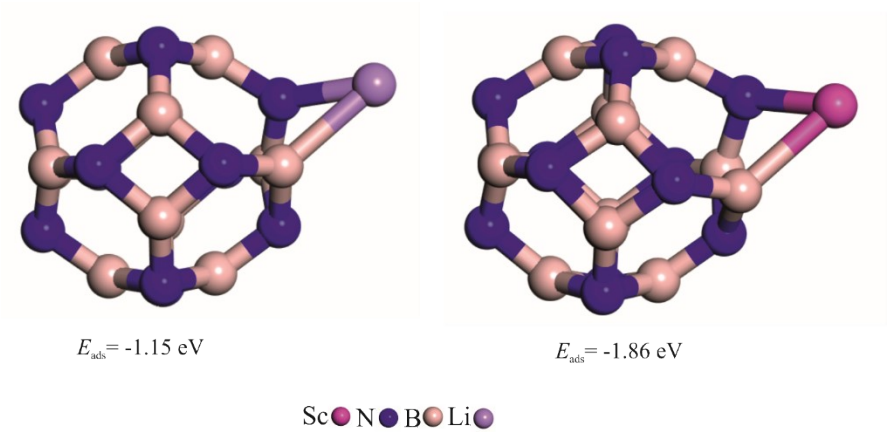

Figure S3. Optimized geometry and adsorption energy of a Li or Sc atom adsorbed on the tetragon ring of $B_{12}N_{11}C$ and $B_{12}C_{12}$ nanocages: (a) $Li@B_{12}N_{11}C$, (b) $Sc@B_{12}N_{11}C$, (c) $Li@B_{12}C_{12}$, and (d) $Sc@B_{12}C_{12}$.

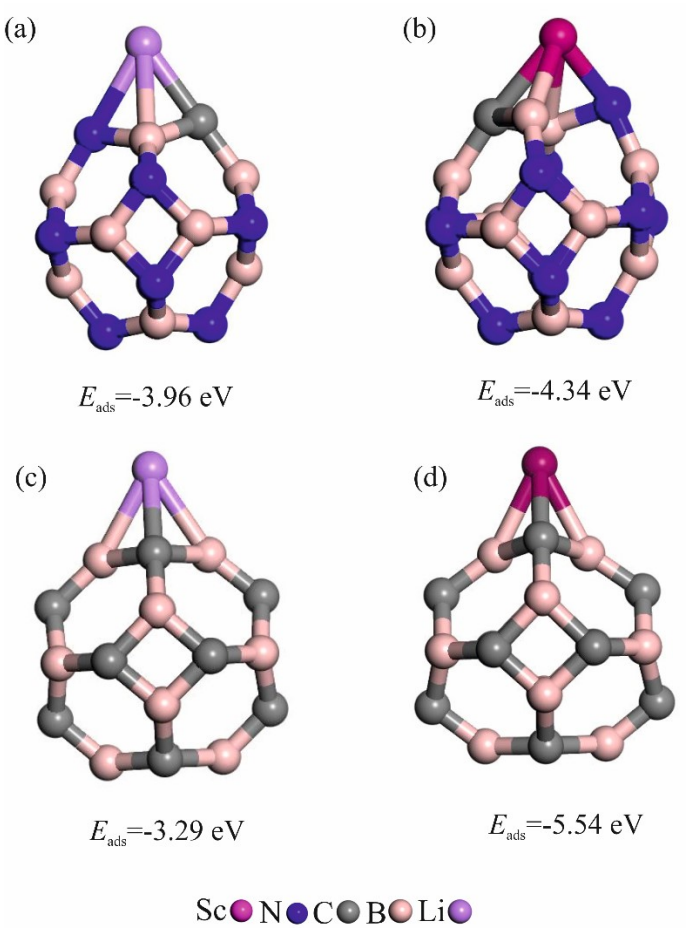

Figure S4. Evolution of the number of adsorbed H_2 molecules as a function of simulation time: (a) $24H_2/Li_8@B_{12}C_{12}$ and (b) $16H_2/Sc_4@B_{12}C_{12}$