Electronic Supplementary Material (ESI) for RSC Advances.

Manipulating Energy Storage Characteristics of Ultrathin Boron Carbide Monolayer Under Varied Scandium Doping

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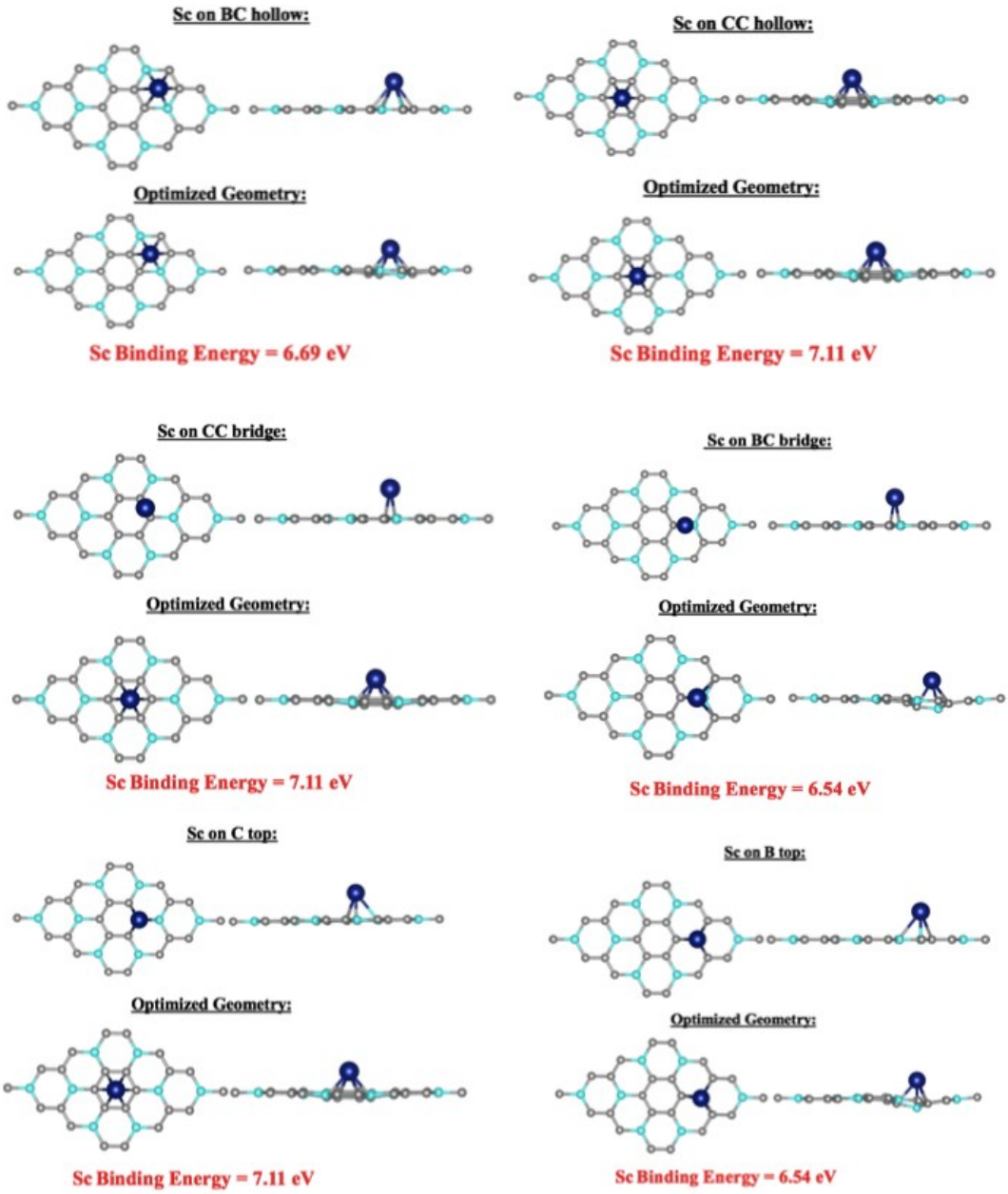
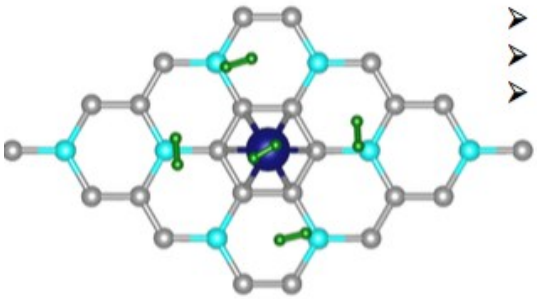
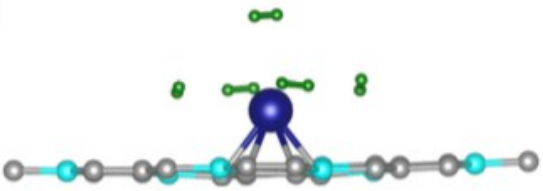


S1 Initial and final geometries of all the possible binding configurations of Sc on BC_3 sheet. Binding energies calculated by van der Waals induced calculations are also given.

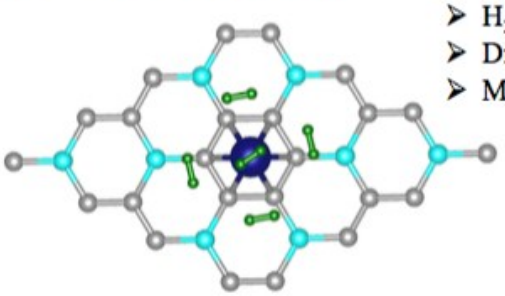
1. Input Geometry:



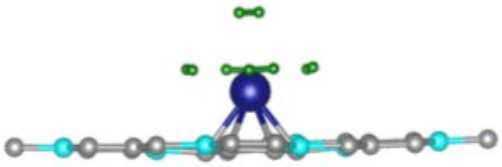
- Horizontally aligned H_2 around Sc
- Distance (Sc-H_2) : 2.80 Å
- Minimum distance between BC_3 and H_2= 2.39Å



Optimized Geometry:



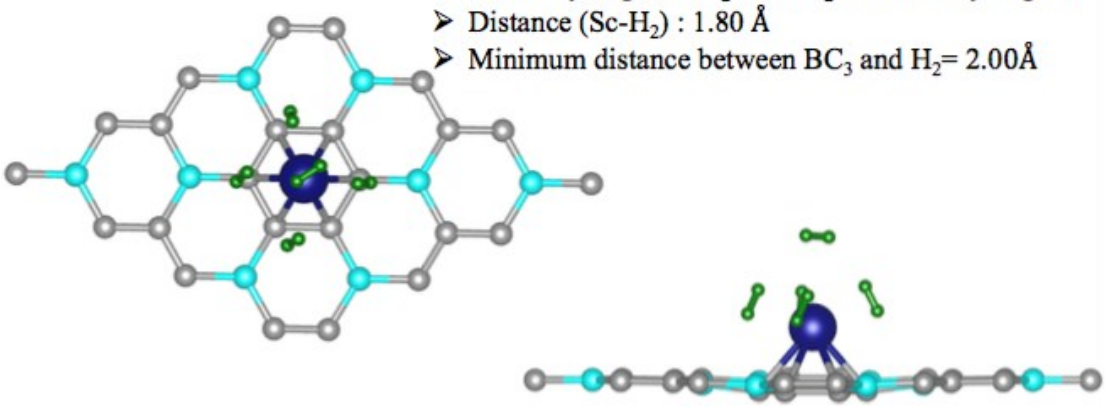
- H_2 stay horizontally aligned around Sc
- Distance (Sc-H_2) : 2.20 Å
- Minimum distance between BC_3 and H_2 = 2.65 Å



H_2 Binding Energy = 0.33 eV

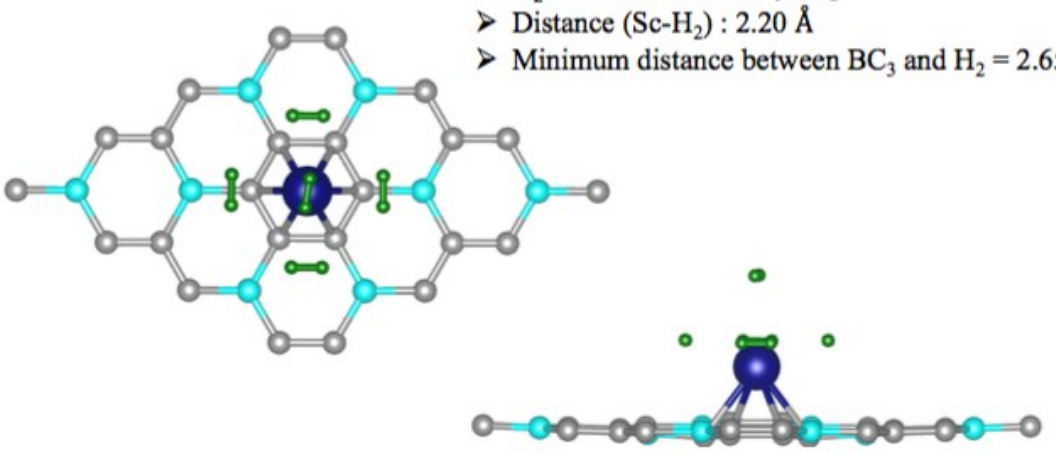
2. Input Geometry:

- Vertically aligned $4H_2$ and $1H_2$ horizontally aligned
- Distance (Sc-H_2) : 1.80 Å
- Minimum distance between BC_3 and H_2= 2.00Å



Optimized Geometry:

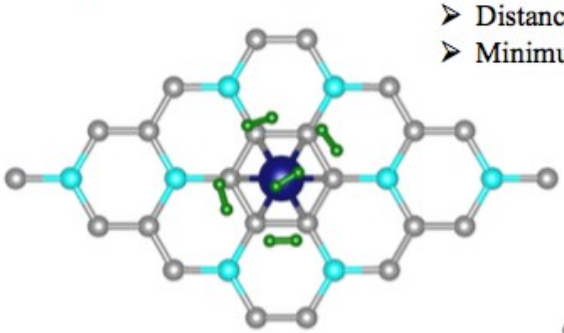
- H_2 become horizontally aligned around Sc
- Distance (Sc-H_2) : 2.20 Å
- Minimum distance between BC_3 and H_2 = 2.65 Å

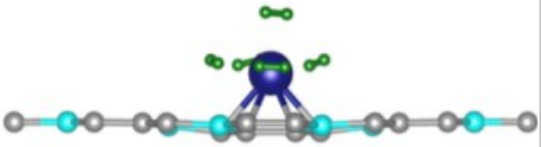


H_2 Binding Energy = 0.34 eV

3. Input Geometry:

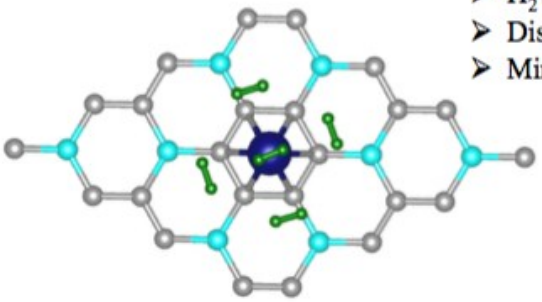
- Horizontally aligned H_2 around Sc
- Distance (Sc-H_2) : 1.80 Å
- Minimum distance between BC_3 and H_2= 2.00 Å

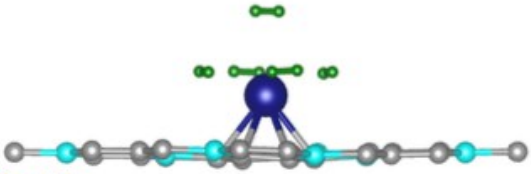




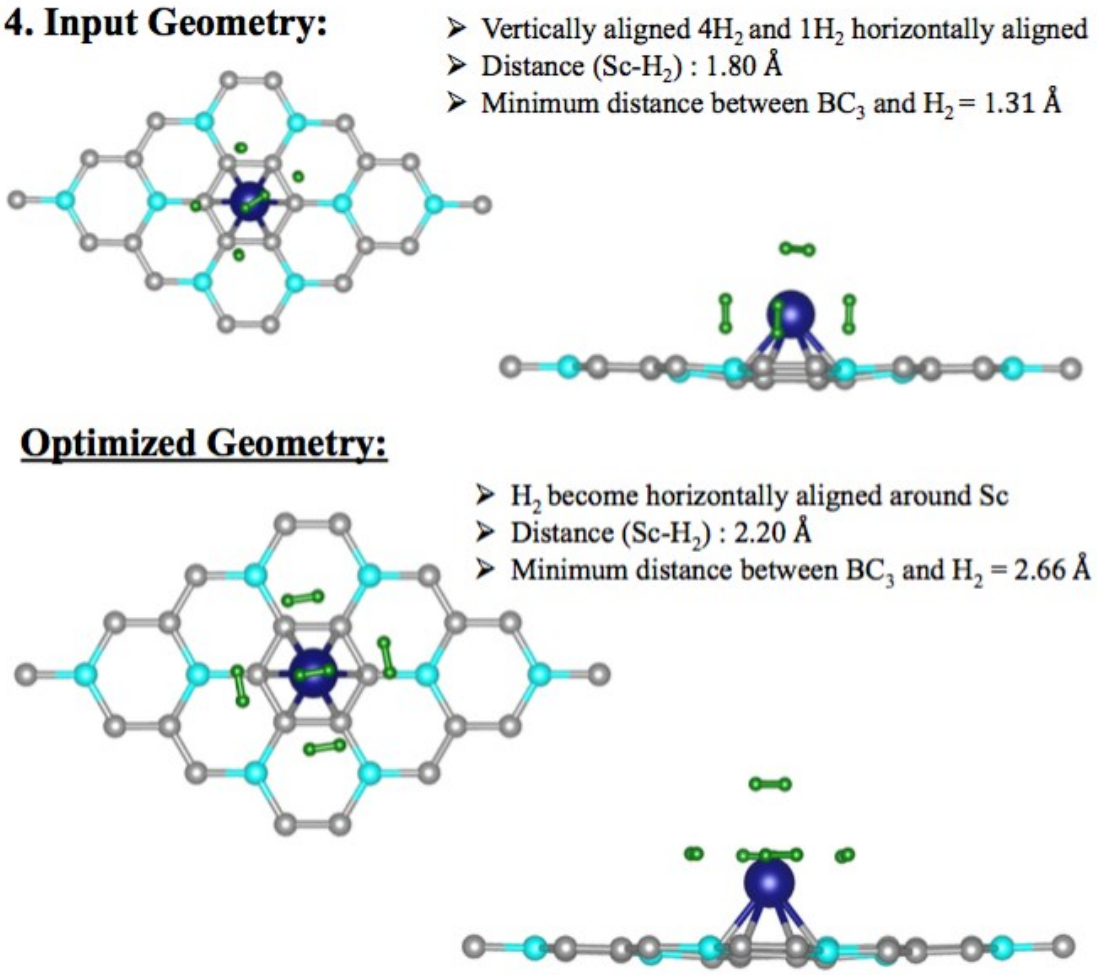
Optimized Geometry:

- H_2 stay horizontally aligned around Sc
- Distance (Sc-H_2) : 2.20 Å
- Minimum distance between BC_3 and H_2 = 2.66 Å

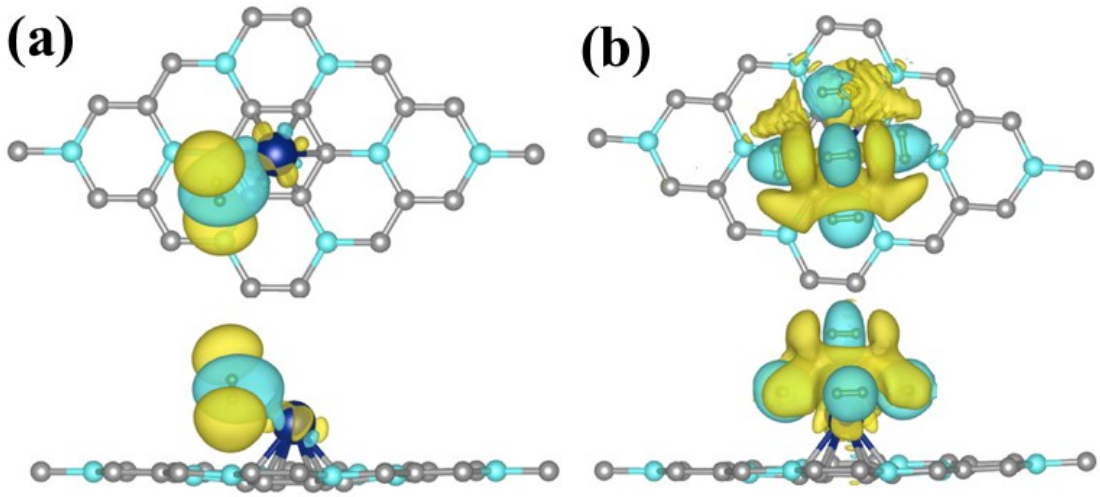




H_2 Binding Energy = 0.34 eV



S2 Initial and final geometries of all the possible binding configurations of H_2 on BC_3@Sc sheet. Adsorption energies calculated by van der Waals induced calculations are also given.



S3 Top and side views of Isosurface charge densities of (a) BC_3@Sc-H_2 and (b) BC_3@Sc-$5H_2$ Cyan and yellow colours indicate the accumulation and depletion of charge respectively.