Supporting Information for

Tuning electronic properties of hydro-boron-carbon compounds by hydrogen and boron contents: a first principles study

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Figure S1:

the convergence with respect to the k-point sampling for BC_3 sheet.

Figure S2:

the convergence with respect to the plane-wave cutoff energies for BC_3 sheet.

Figure S3:

the convergence with respect to the k-point sampling for all-H type of hydro-BC_3 compound.

Figure S4:

the convergence with respect to the plane-wave cutoff energies for all-H type of hydro-BC_3 compound.

Figure S5:

The energy bands of BC_3 sheet and hydro-BC_3 compounds by PAW pseudopotentials.

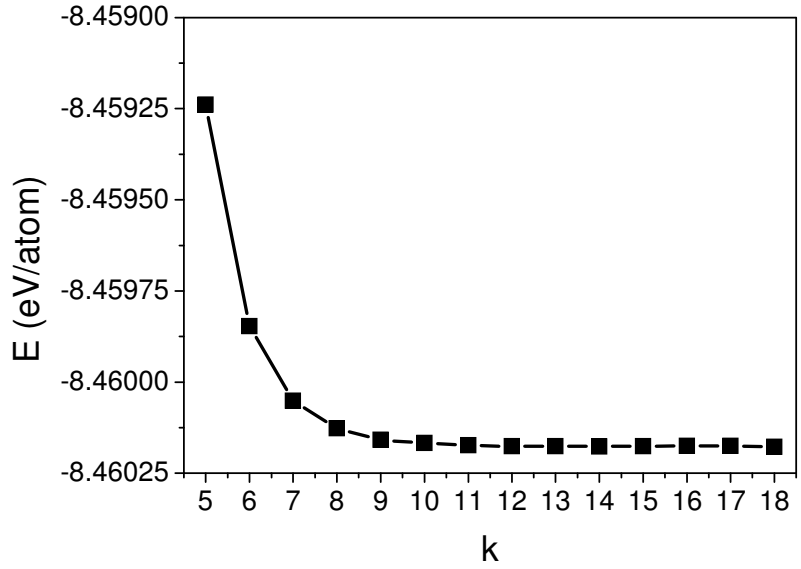

Figure S1: The total energies of BC_3 sheet versus different $k \times k \times 1$ k-mesh. The plane-wave cutoff energy is fixed as 350 eV.

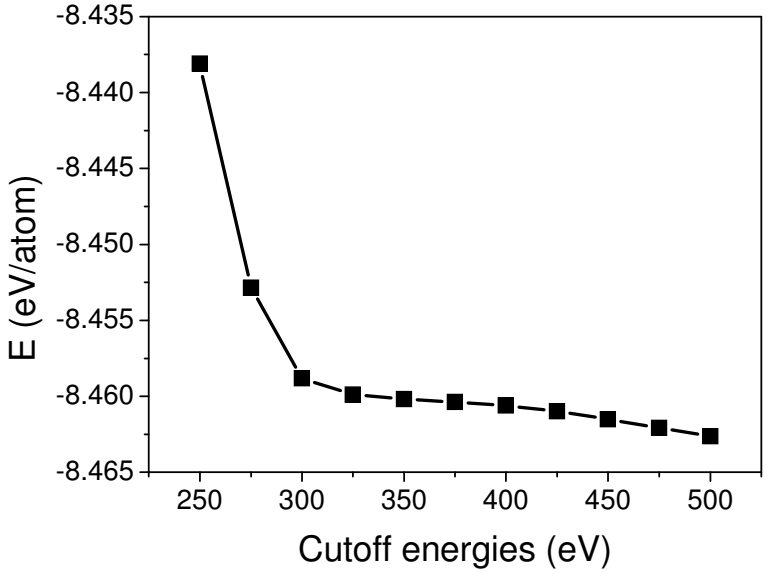

Figure S2: The total energies of BC_3 sheet versus different plane-wave cutoff energies. The k-mesh is fixed as $15 \times 15 \times 1$.

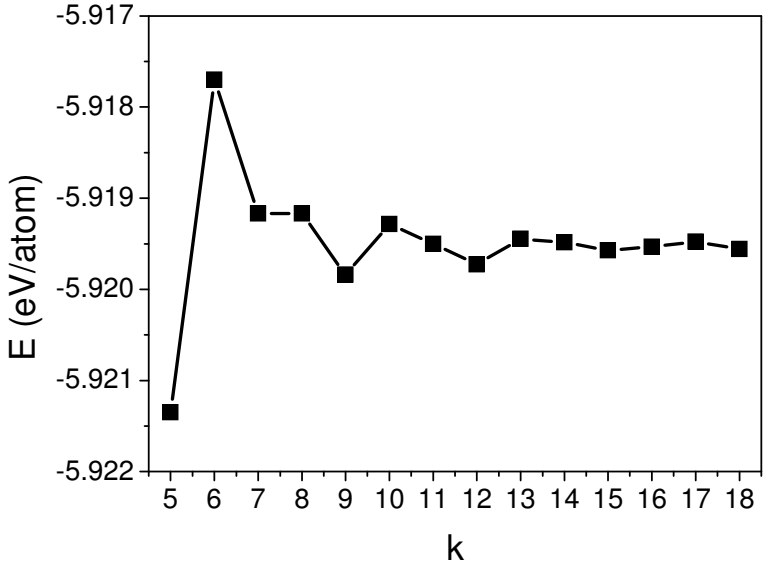

Figure S3: The total energies for all-H type of hydro-BC_3 compound versus different $k \times k \times 1$ k-mesh. The plane-wave cutoff energy is fixed as 350 eV.

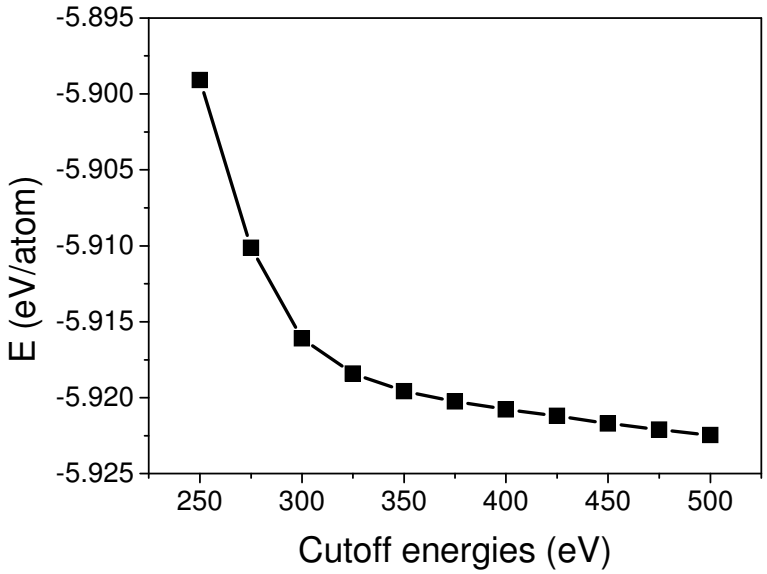

Figure S4: The total energies for all-H type of hydro-BC_3 compound versus different plane-wave cutoff energies. The k-mesh is fixed as $15 \times 15 \times 1$.

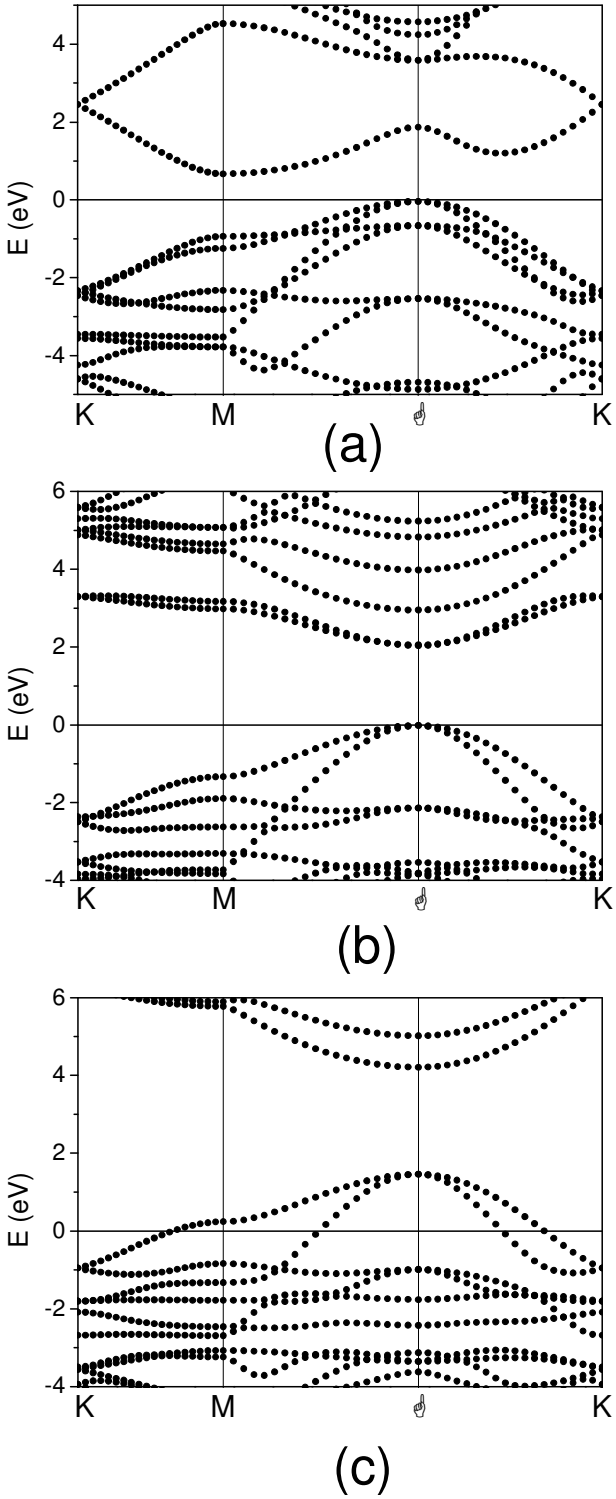

Figure S5: The energy bands of (a) the BC_3 sheet, (b) the C-H type and (c) the all-H type of hydro-BC_3 compounds. The Fermi level is indicated as the line at E =0.0 eV.