Electronic supplementary information for

Boron position-dependent surface reconstruction and electronic states of boron-doped diamond (111) surfaces: an *ab initio* study

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1.1. Revisit of the diamond (100) surface reconstructions

Table S1. Calculated surface energies of the unterminated, monohydride, and dihydride (100) surfaces.

Surfaces	E_s (eV/site)
(100)-p(2x1):0H	2.91
(100)-c(2x2):0H	3.01
(100)-p(2x1):1H	0.97
(100)-c(2x2):1H	1.14
(100)-tilted:2H	2.05

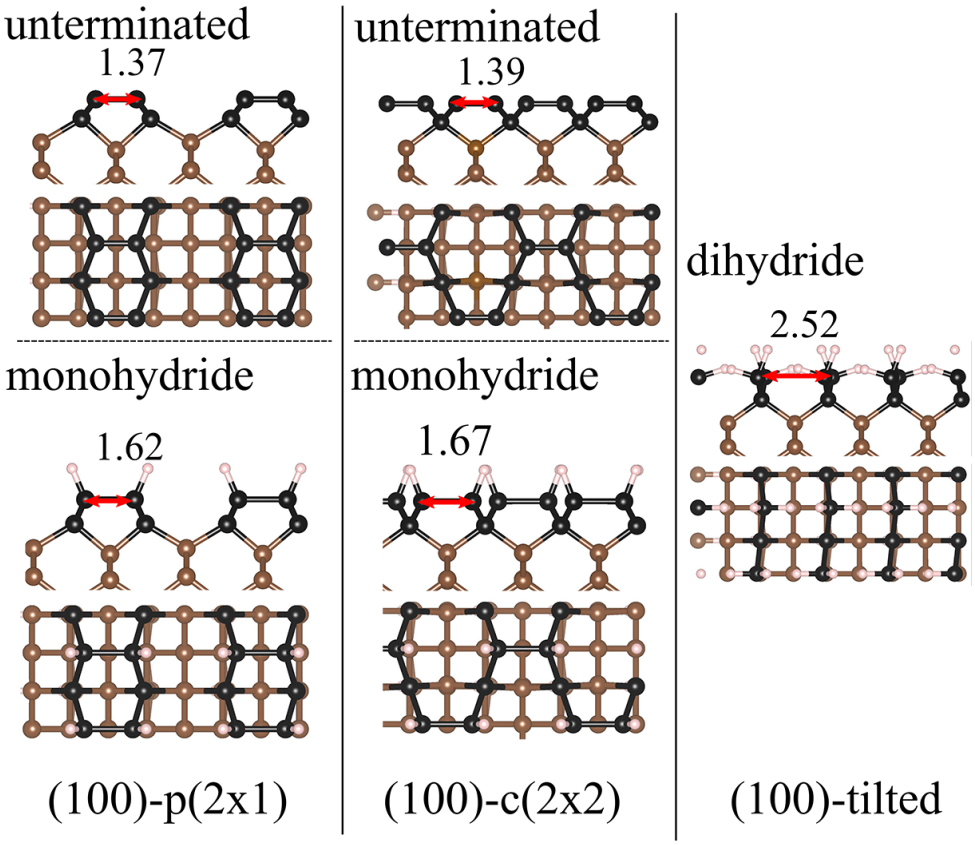

Figure S1. Atomistic reconstructions of the diamond (100) surfaces with unterminated, monohydride and dihydride terminations. The surface Carbon atoms are black while the others are brown. The Hydrogen atoms are white balls. The values are bond lengths in (Å).

1.2. The projected density of states of the (100) surfaces

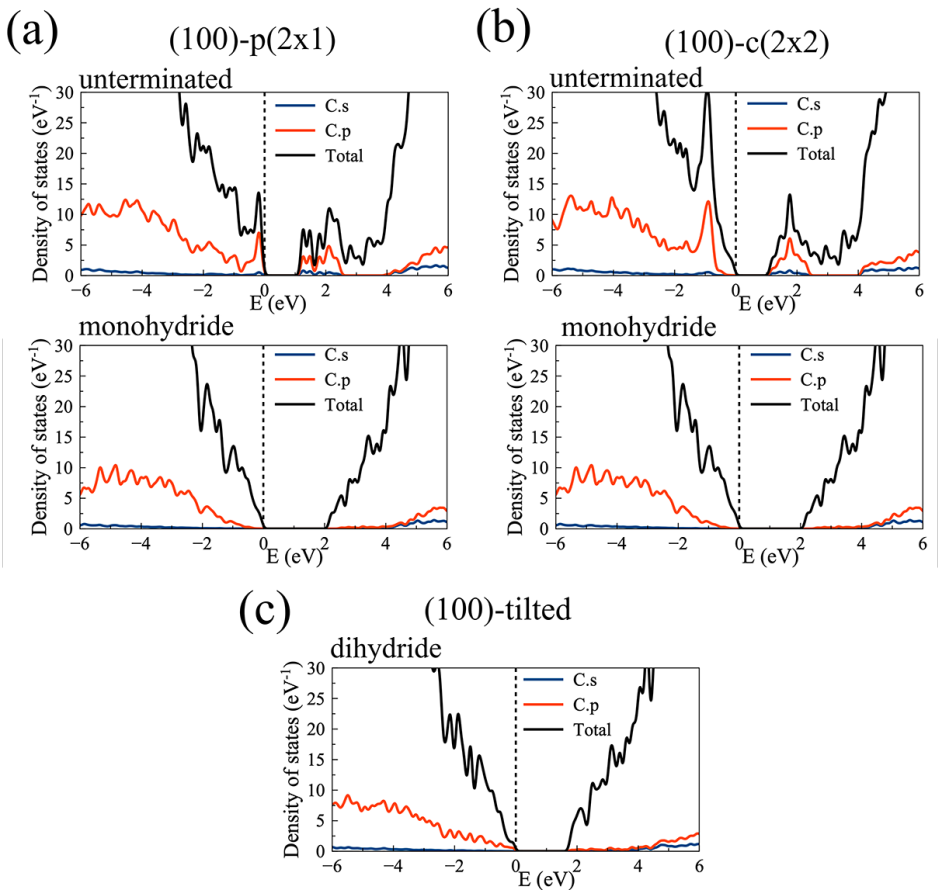

Figure S2. Projected density of states (PDOS) for the (a) (100)-p(2x1), (b) (100)-c(2x2), and (100)-tilted surfaces with different H-terminations: unterminated, monohydride 1H, and dihydride 2H. The total DOS is plotted together with *s*-, and *p*-revolved orbital PDOS of the surface Carbon atoms. The origin of energy is set at the highest occupied state.

2. Surface energies and density of states of the unterminated Pandey chain (111)-(1x1)-PC:0H and single chain (111)-(1x1)-SC:0H

Table S2. Calculated surface energies of the unterminated Pandey chain (111)-(2x1)-PC:0H and single chain (111)-(2x1)-SC:0H surfaces

Surfaces	(111)-(2x1)-PC:0H E_s (eV/site)	(111)-(2x1)-SC:0H E_s (eV/site)
Undoped	0.38	2.02
B at layer 1	0.31	1.74
B at layer 2	0.32	1.75
B at layer 3	0.34	1.77
B at layer 4	0.34	1.91
B at layer 5	0.34	1.96
B at layer 6	0.36	1.98
B at layer 7	0.36	1.99

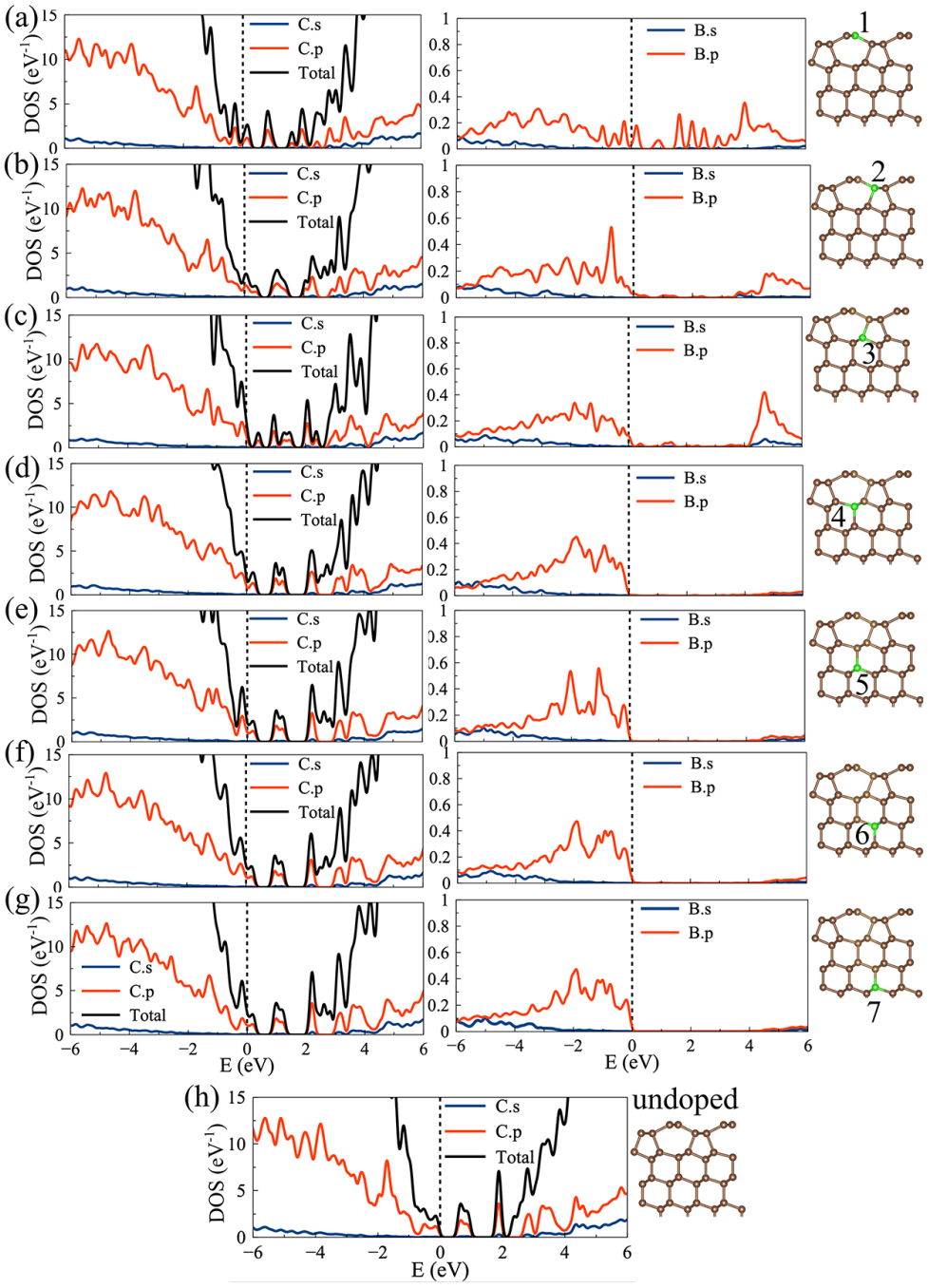

Figure S3. Density of states of the unterminated B-doped Pandey chain (111)-(2x1)-PC:0H surfaces (a-g) in comparison with the undoped case (h). The position of the Boron atom (green ball) is changed from the 1st layer (a) to the 7th layer (g). The origin of energy is set at the highest occupied state.

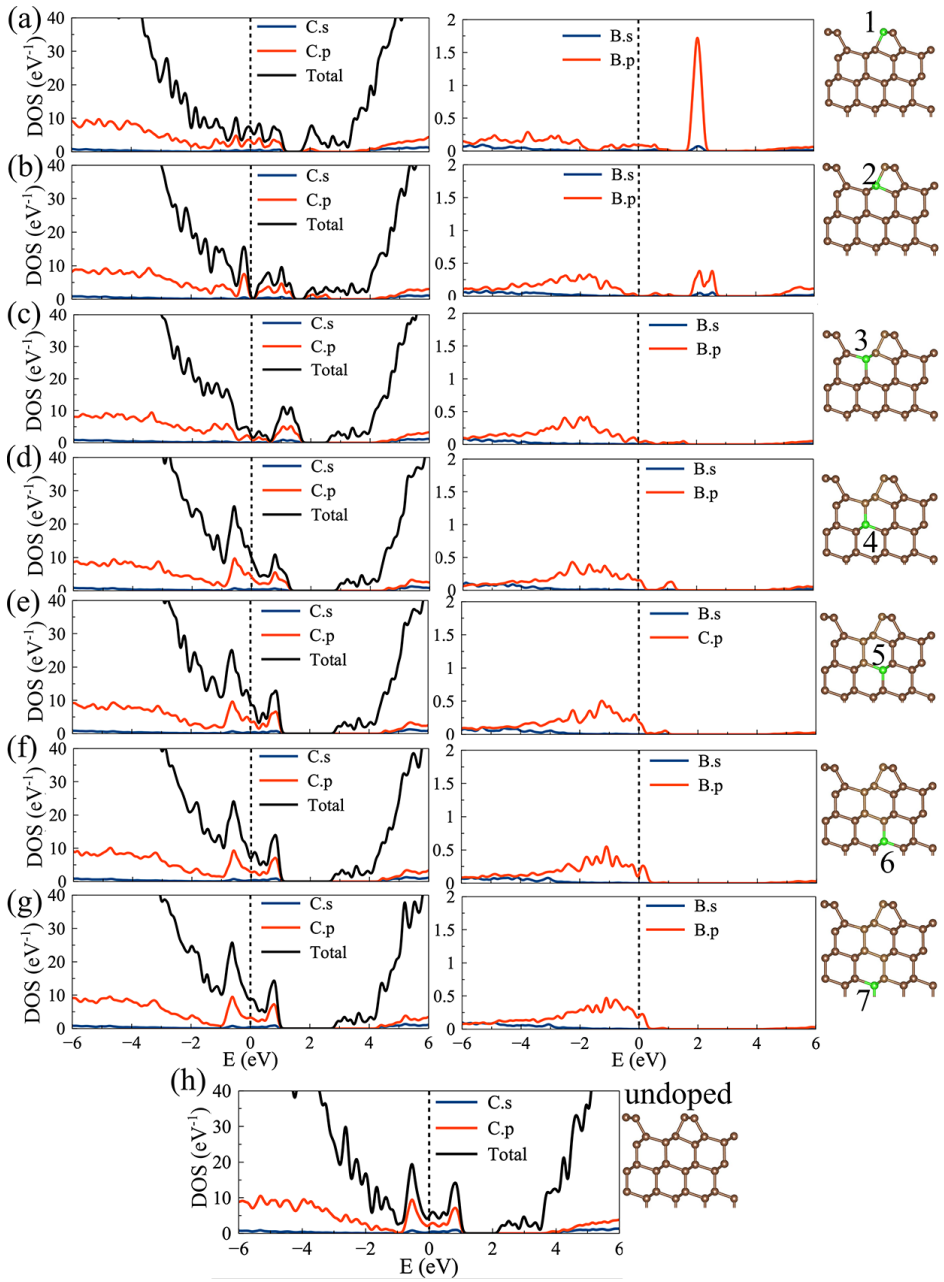

Figure S4. Density of states of the unterminated B-doped single chain (111)-(2x1)-SC:0H surfaces (a-g) in comparison with the undoped case (h). The position of the Boron atom (green ball) is changed from the 1st layer (a) to the 7th layer (g). The origin of energy is set at the highest occupied state.

3. Surface energies and density of states of the H-terminated pristine (111)-(1x1):1H, Pandey chain (111)-(1x1)-PC:1H and single chain (111)-(1x1)-SC:1H and (111)-(1x1)-SC:2H

Table S3. Calculated surface energies of the H-terminated BDD (111) surfaces

Surfaces	pristine (1x1):1H E_s (eV/site)	PC:1H E_s (eV/site)	SC:1H E_s (eV/site)	SC:2H E_s (eV/site)
Undoped	-0.79	-0.13	-0.44	0.33
B at the 1st layer	-0.68	-0.16	-0.42	0.32
B at the 2nd layer	-0.77	-0.22	-0.43	0.31
B at the 3rd layer	-0.79	-0.11	-0.47	0.31
B at the 4th layer	-0.79	-0.16	-0.47	0.31
B at the 5th layer	-0.79	-0.16	-0.44	0.32
B at the 6th layer	-0.79	-0.13	-0.45	0.32
B at the 7th layer	-0.80	-0.13	-0.44	0.32

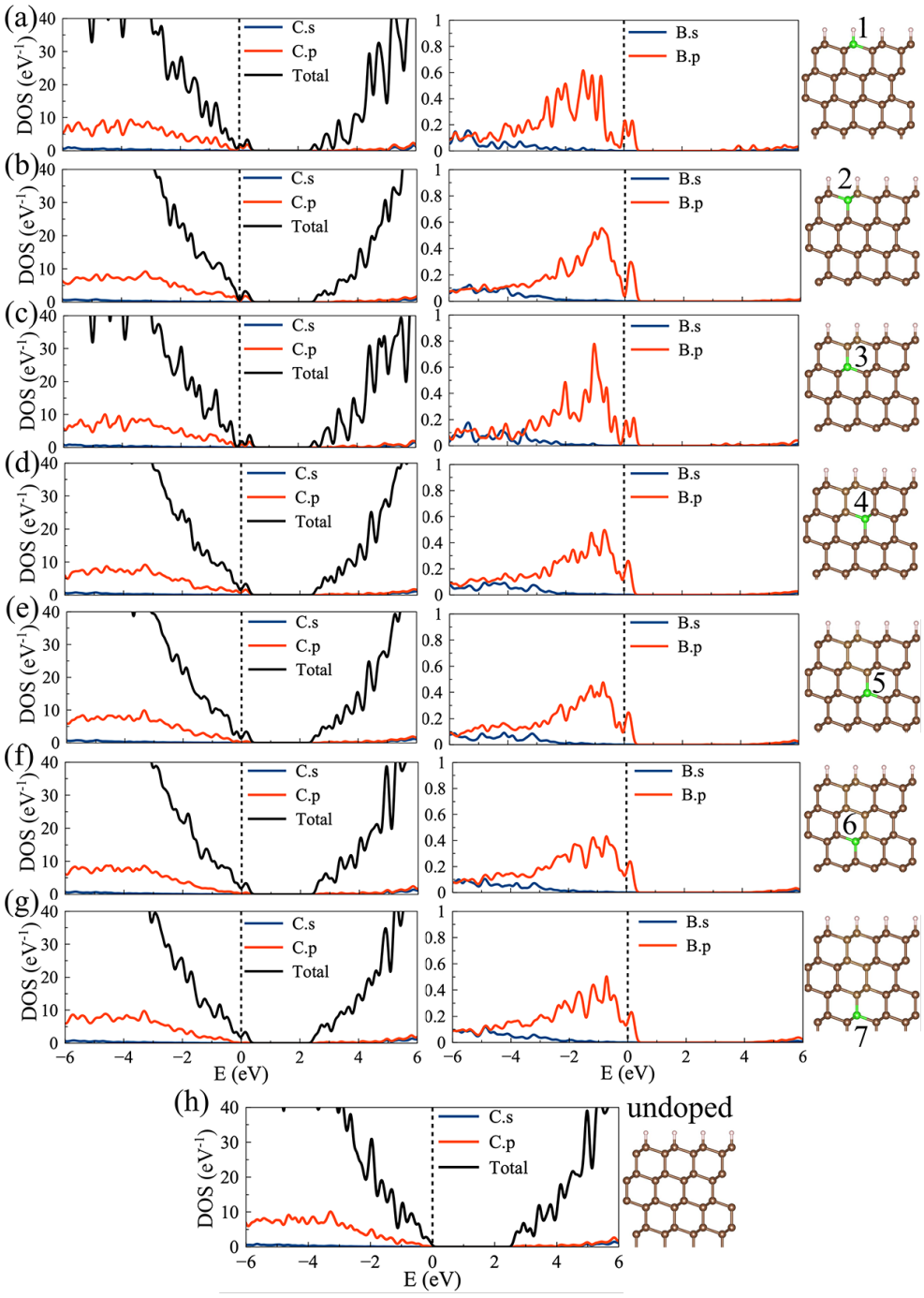

Figure S5. Density of states of the monohydride pristine (111)-(1x1):1H surfaces (a-g) in comparison with the undoped case (h). The position of the Boron atom (green ball) is changed from the 1st layer (a) to the 7th layer (g). The origin of energy is set at the highest occupied state.

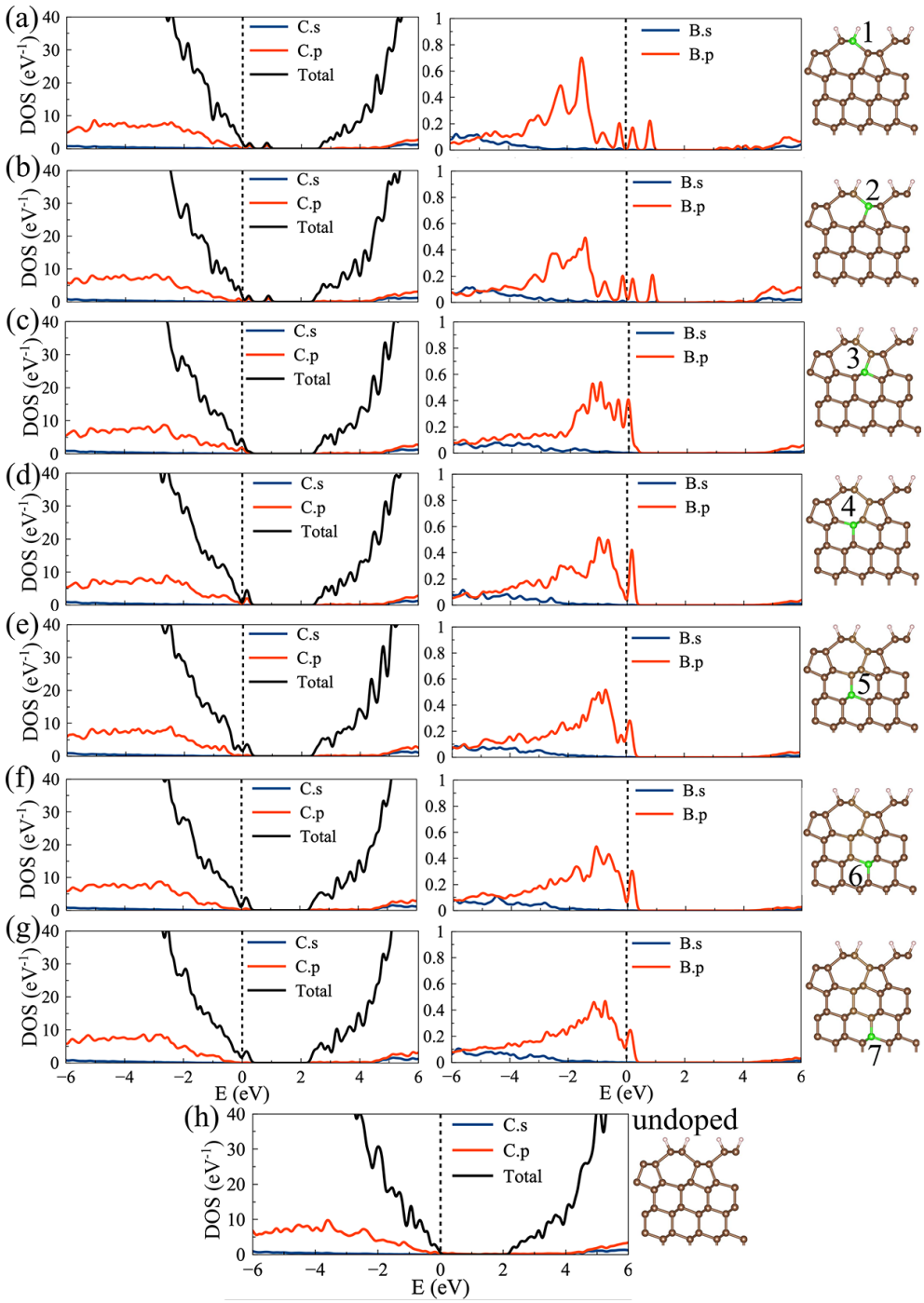

Figure S6. Density of states of the monohydride Pandey chain (111)-(2x1)-PC:1H surfaces (a-g) in comparison with the undoped case (h). The position of the Boron atom (green ball) is changed from the 1st layer (a) to the 7th layer (g). The origin of energy is set at the highest occupied state.

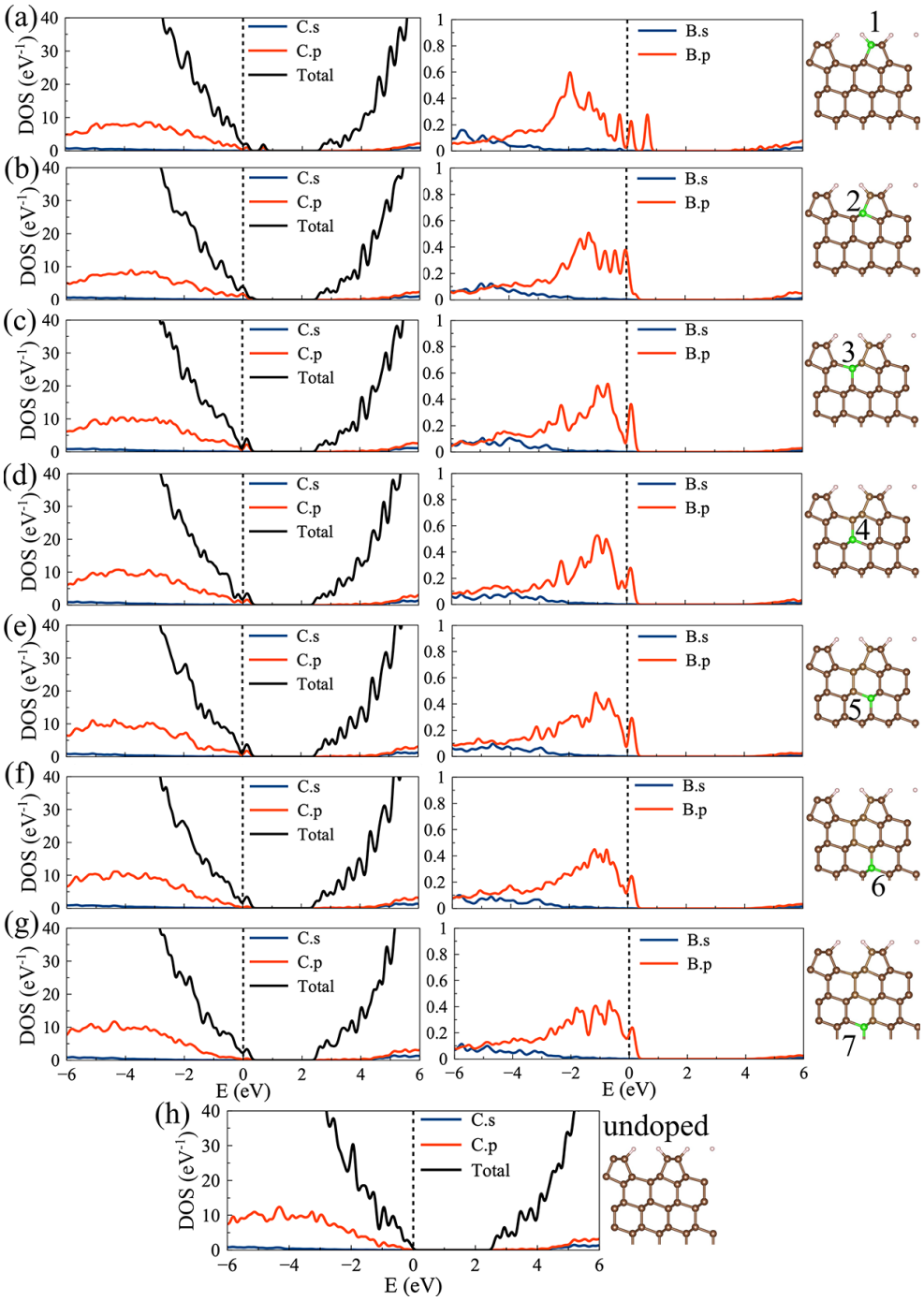

Figure S7. Density of states of the monohydride single chain (111)-(2x1)-SC:1H surfaces (a-g) in comparison with the undoped case (h). The position of the Boron atom (green ball) is changed from the 1st layer (a) to the 7th layer (g). The origin of energy is set at the highest occupied state.

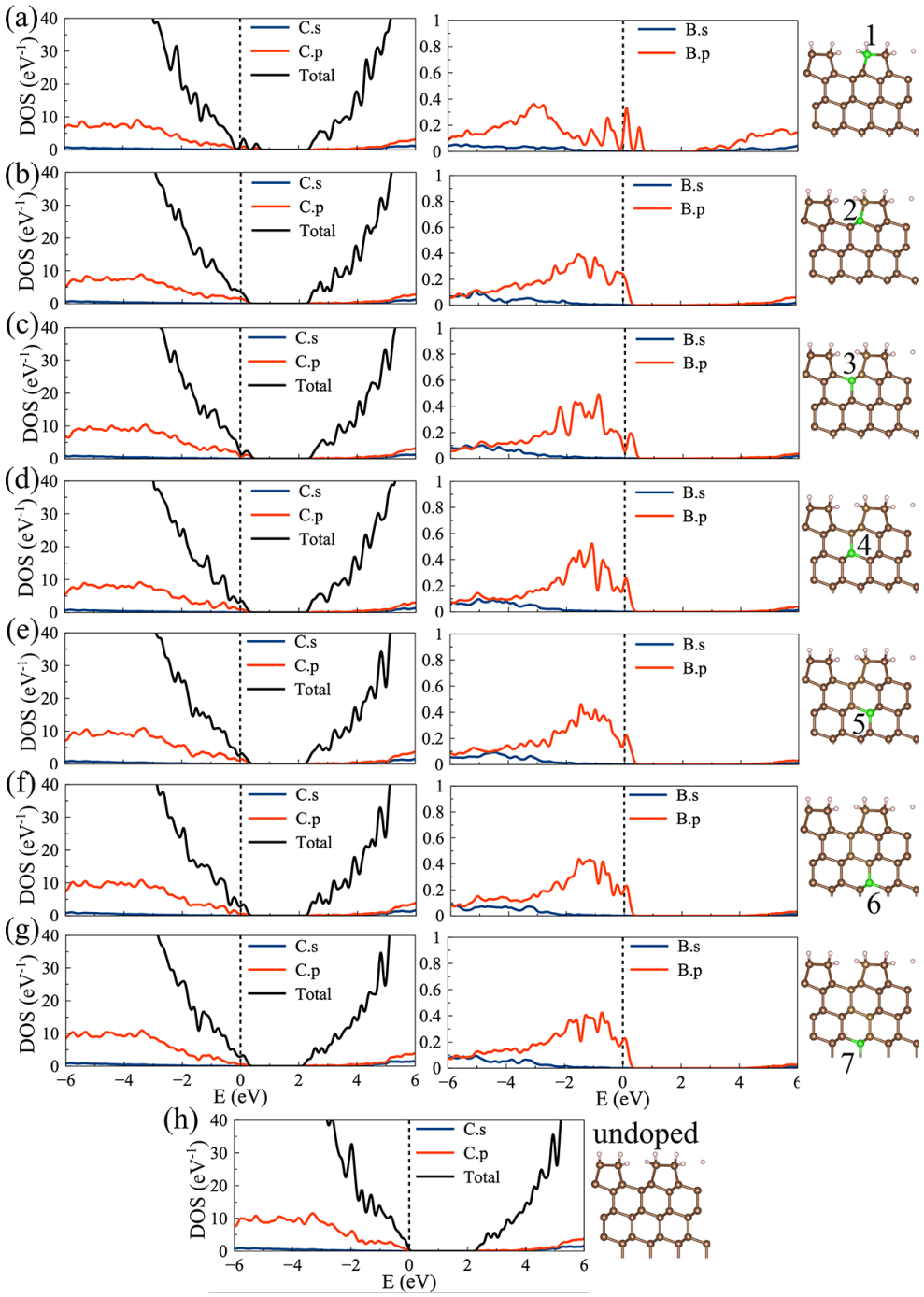

Figure S8. Density of states of the dihydride single chain (111)-(2x1)-SC:2H surfaces (a-g) in comparison with the undoped case (h). The position of the Boron atom (green ball) is changed from the 1st layer (a) to the 7th layer (g). The origin of energy is set at the highest occupied state.

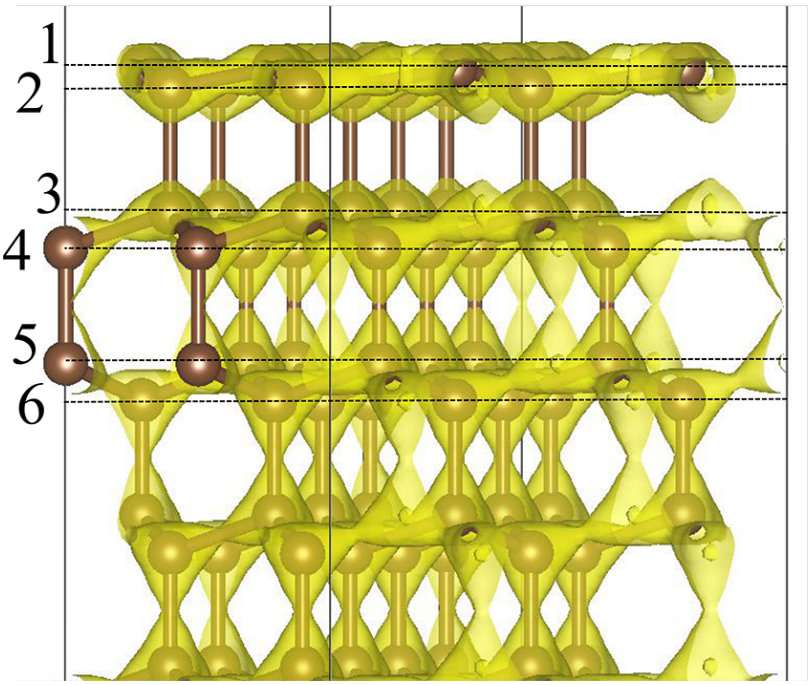

Figure S9. The 3D view of total charge density distribution in the (111)-(1x1):0H surface. The iso-value is set at 0.21 (e/Bohr^3). The numbers indicate the order of the layers from the topmost.