Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

for

Boron-terminated diamond (100) surfaces with promising structural and electronic properties

Zhaolong Sun, Mingchao Yang, Xueting Wang, Peng Wang, Chunling Zhang, Nan Gao,*

Hongdong Li*

State Key Lab of Superhard Materials, College of Physics, Jilin University, Changchun 130012, PR China

Corresponding Authors

Email address: hdli@jlu.edu.cn, gaon@jlu.edu.cn

Fig. S1 of 3

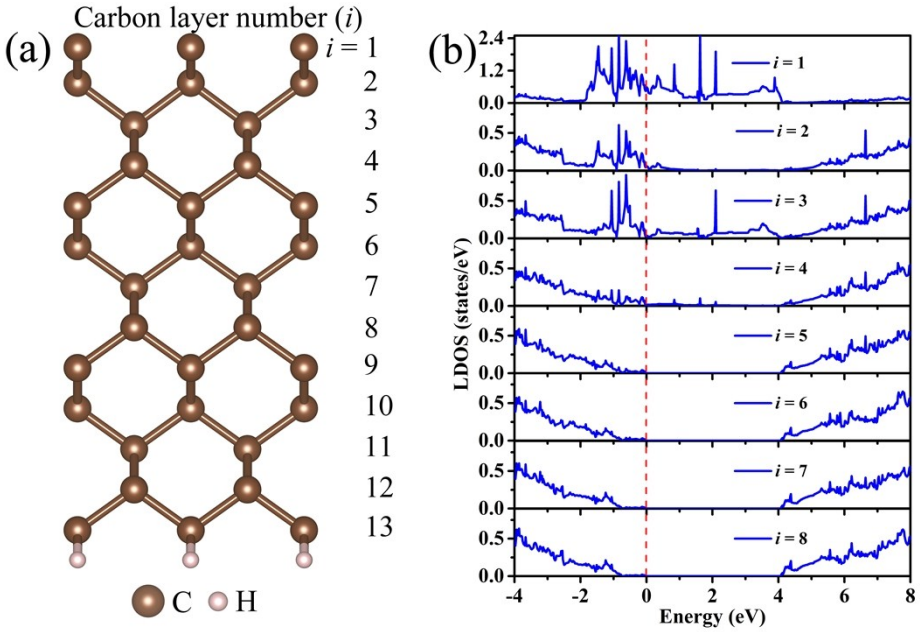

Fig. S1 (a) The ideal asymmetric slab for H-terminated diamond (100) surface structure, and each carbon layer number is labeled. The grey and pink balls represent the C and H atoms, respectively. (b) Layer-by-layer local density of states (LDOS) (i =1 to 8) are taken from the outmost layer on one side to the opposite side in turn. The Fermi level is set to zero.

To test the influence of layer thickness on the structure prediction, we build up an asymmetric diamond (100) slab with the bare carbon layer on top side and the opposite bottom side passivated by hydrogen atoms. The slab with 13 carbon layers is first chosen, and the bottom 5 layers with hydrogenation are fixed with pristine diamond structure, and the upper 8 layers are allowed to be relaxed for structural optimization. The layer numbers are labeled as i = 1 to 13 from the outmost unsaturated side to the opposite side in turn (Fig. S1a). The local density of states (LDOS) of each layer from i = 1 to 8 calculated are shown in Fig. S1b. Near the outside layers (from i=1 to 4), there are DOS levels appearing in the band gap, meaning the presences of the surface levels. With the increase of diamond surface thickness up to 5th layer and more layers, no DOS levels appear in band gap of each layer, and the band structure tends to be constant as that of bulk diamond. Thus, we consider a 10-layer-thick diamond (100) surface model in the structure search, the 5 carbon layers on the bottom side are fixed to maintain the bulk diamond, and the upper 5 carbon layers are allowed to be relaxed.

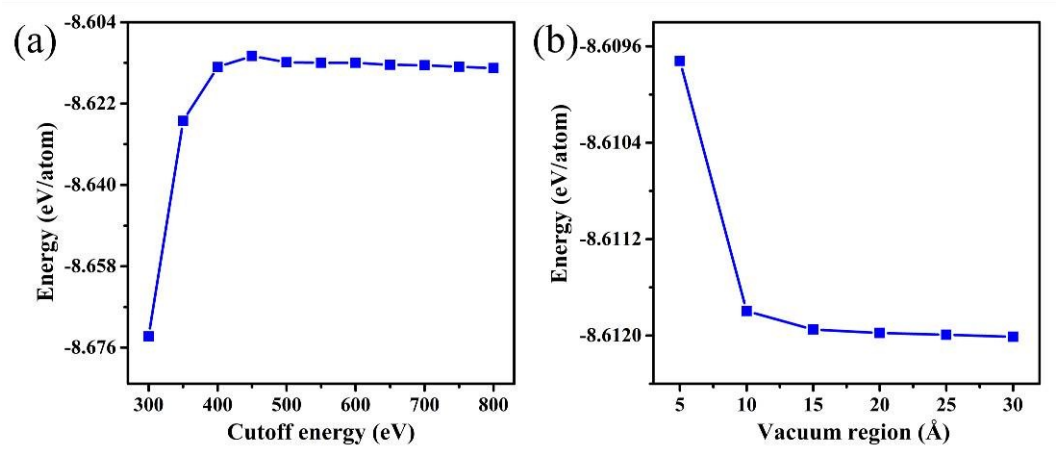

Fig. S2 Convergence tests of the asymmetric slab dependent on the variation of cutoff energy (a) and slab separation (b).

The convergence standard is smaller than 1 meV/atom, when the cutoff energy (vacuum layer thickness) is selected as 500 eV (15 Å). It safely concludes that cutoff energy and vacuum layer selected in the paper is reasonable for the calculations.

Fig. S3 of 3

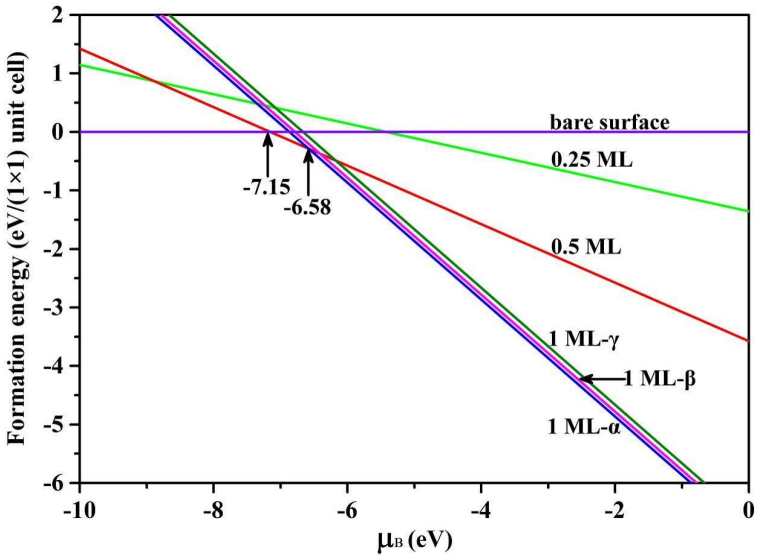

Fig. S3 The surface formation energy for bare diamond (100) surface and B-terminated diamond (100) surfaces with 0.25 ML, 0.5 ML, 1 ML-α, 1 ML-β, and 1 ML-γ coverages as a function of B chemical potential.