**Supporting Information**

for

# Structural and electronic properties of pristine and hydrogen-terminated c-BN (100) surfaces

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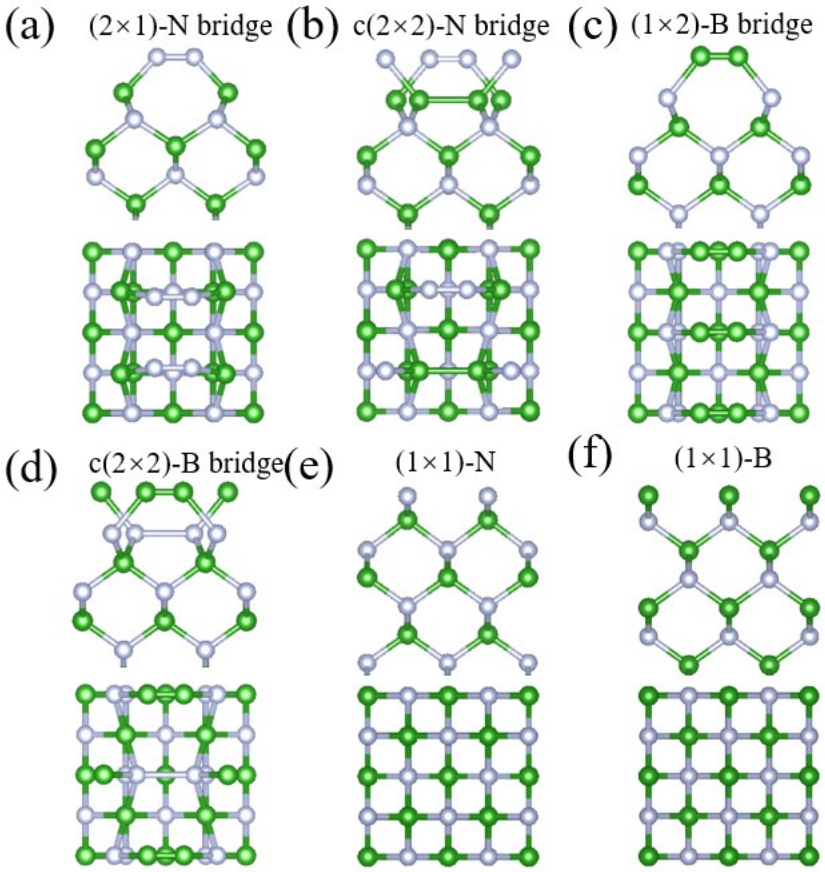


Fig. S1 Top and side views of pristine c-BN (100) surface with (a) (2×1)-N bridge, (b) c(2×2)-N bridge, (c) (1×2)-B bridge, (d) c(2×2)-B bridge, (e) (1×1)-N, and (f) (1×1)-B configurations. The green and grey balls represent B and N atoms, respectively.

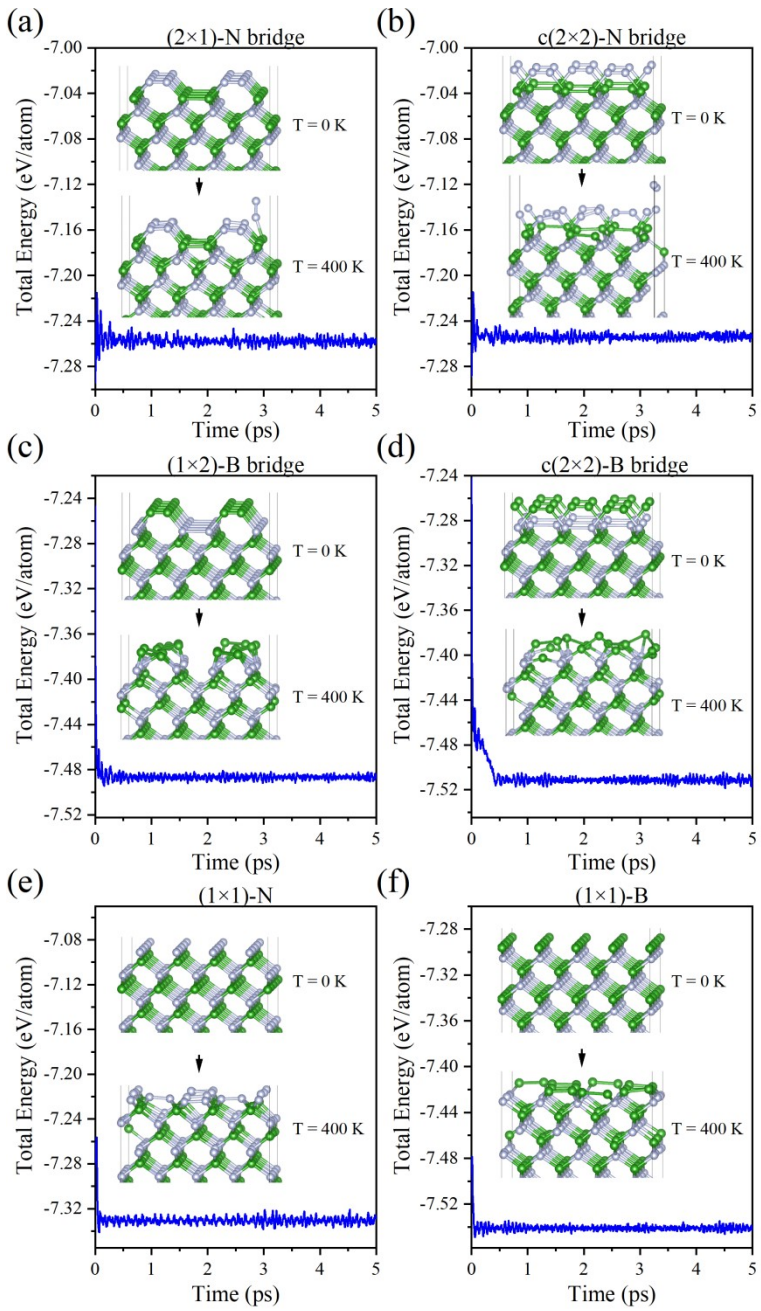


Fig. S2 AIMD evolutions of total energy of pristine c-BN (100) surface with (a) (2×1)-N bridge, (b) c(2×2)-N bridge, (c) (1×2)-B bridge, (d) c(2×2)-B bridge, (e) (1×1)-N, and (f) (1×1)-B configurations. The insets show the equilibrium structures at 0 K and 400 K after 5 ps with a time step of 1 fs AIMD simulations. The green and grey balls represent B and N atoms, respectively.

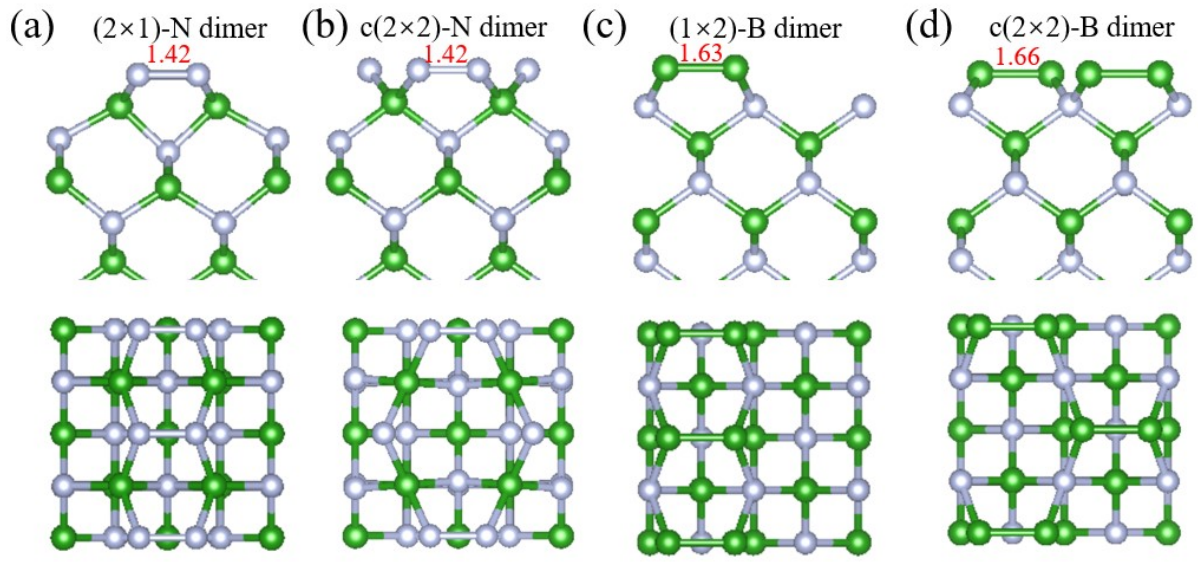


Fig. S3 Top and side views of pristine c-BN (100) surface with (a) (2×1)-N dimer, (b) c(2×2)-N dimer, (c) (1×2)-B dimer and (d) c(2×2)-B dimer configurations. The green and grey balls represent B and N atoms, respectively.

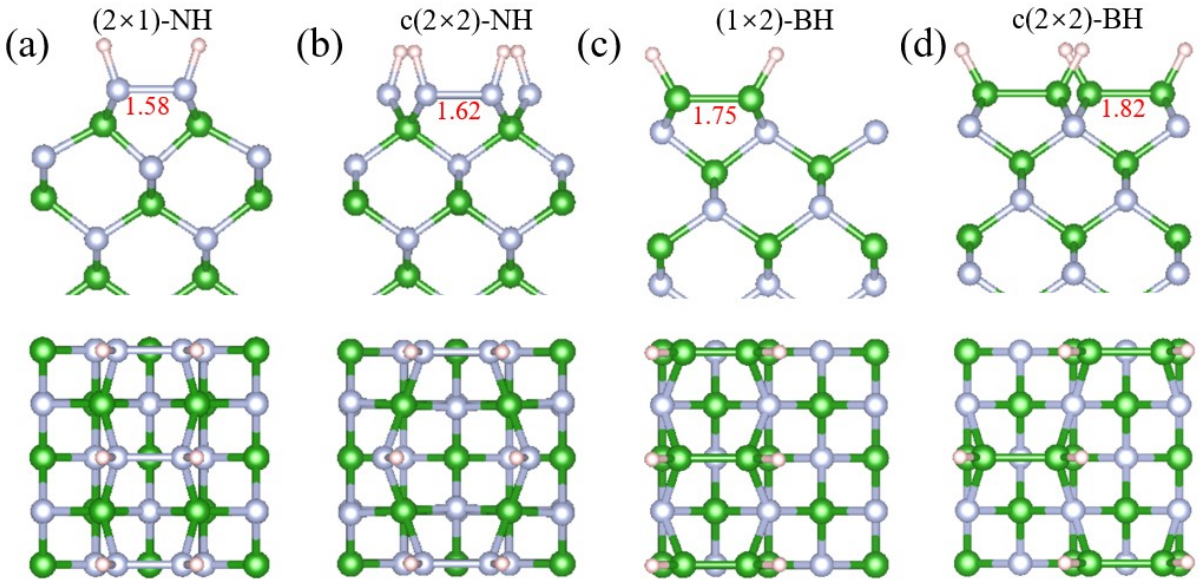


Fig. S4 Top and side views of H-terminated c-BN (100) surface with (a) (2×1)-NH, (b) c(2×2)-NH, (c) (1×2)-BH and (d) c(2×2)-BH configurations. The green, grey and pink balls represent B, N and H atoms, respectively.

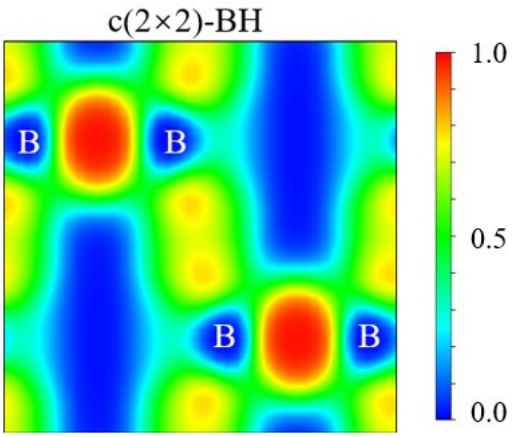


Fig. S5 Top view of the electron localization functions (ELFs) for the c(2×2)-BH dimer structure, and the blue to red indicates the gradually increased charge localization.

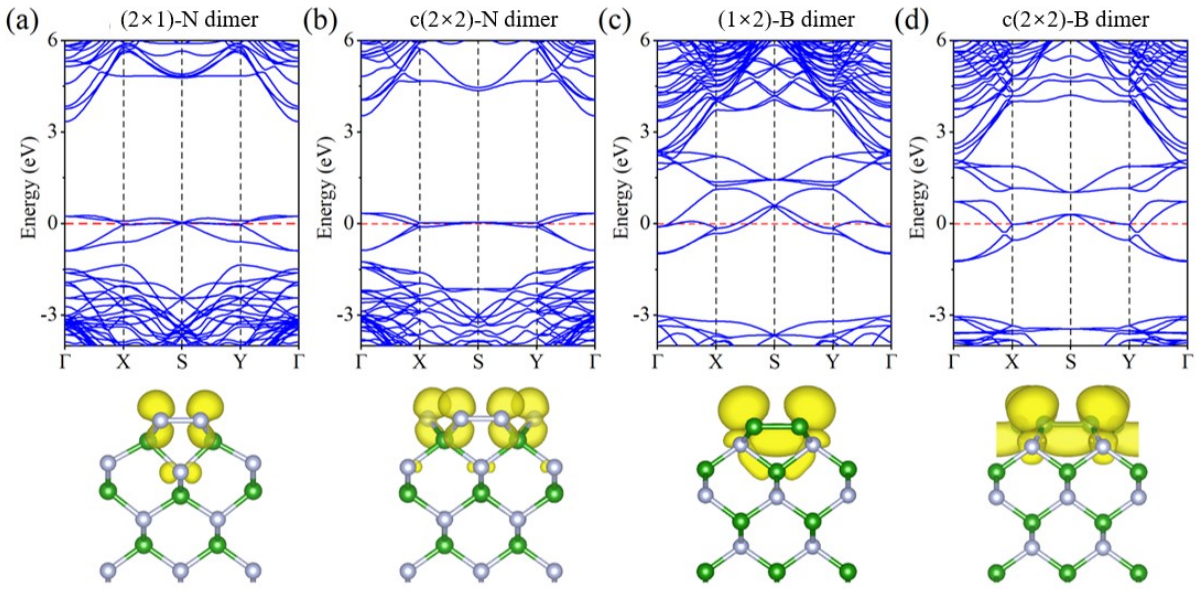


Fig. S6 The band structures and charge densities for pristine c-BN (100) surface of the bands near the Fermi energy with (a) (2×1)-N dimer, (b) (2×2)-N dimer, (c) (1×2)-B dimer and (d) c(2×2)-B dimer structures. The isovalue is 0.001 e $Å^{-3}$. The green and grey balls represent B and N atoms, respectively.

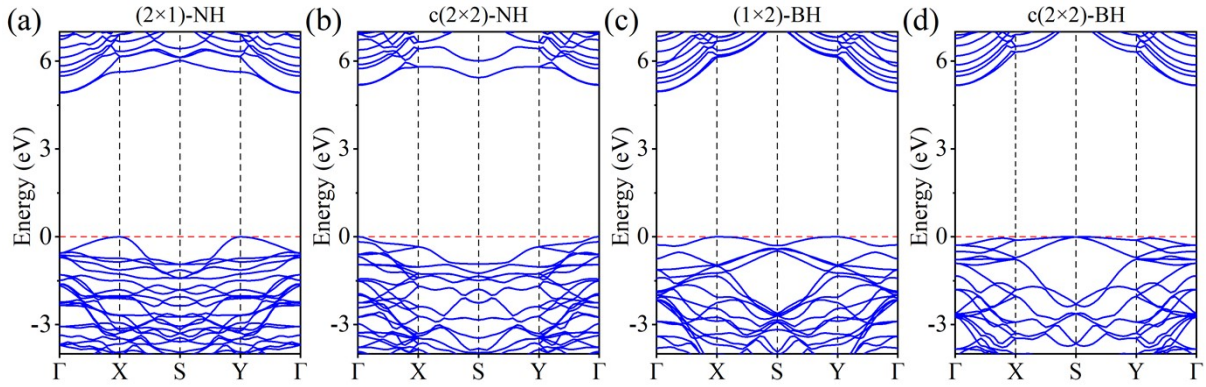


Fig. S7 Electronic band structures of H-terminated c-BN (100) surfaces with (a) (2×1)-NH, (b) c(2×2)-NH, (c) (1×2)-BH, and (d) c(2×2)-BH structures by HSE06 functional.

The band gap values for H-terminated c-BN (100) surfaces in HSE06 functional increase to 4.92 eV, 5.18 eV, 4.96 eV, and 5.17 eV, respectively.