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Highly Anisotropic Gas Sensing of Atom-thin Borophene: A first-principles study

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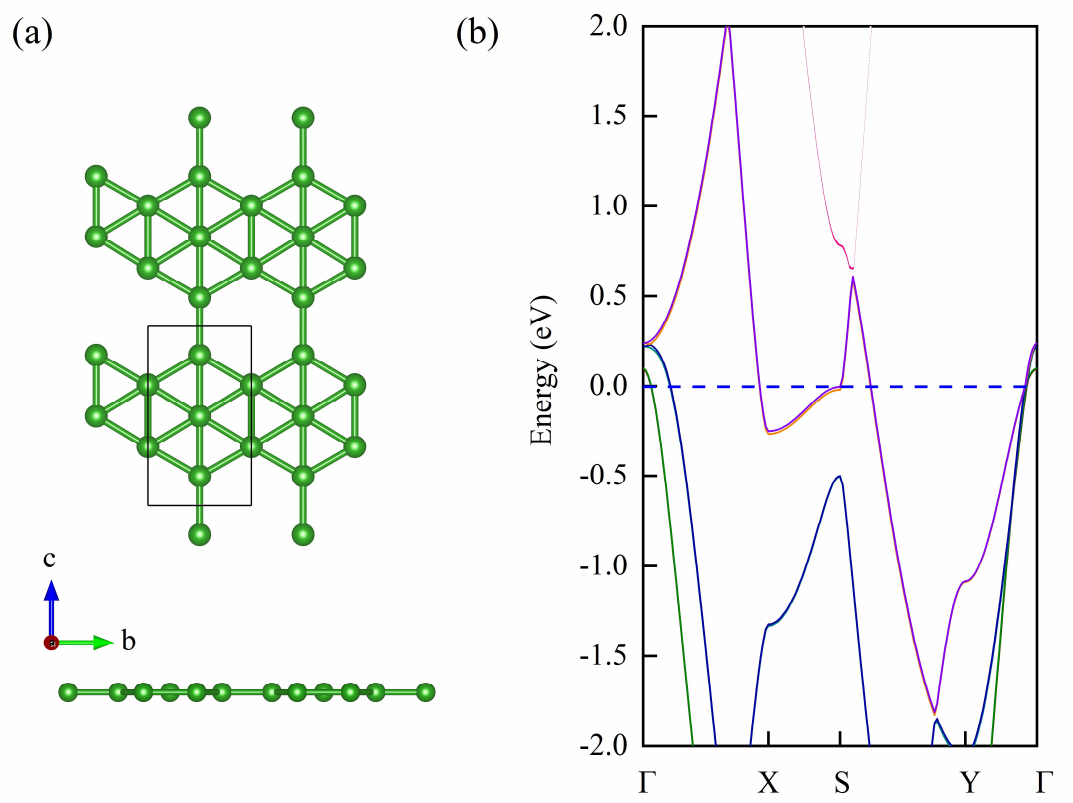

Fig. S1. Top, side view and Energy bands of pristine β_{12} borophene.

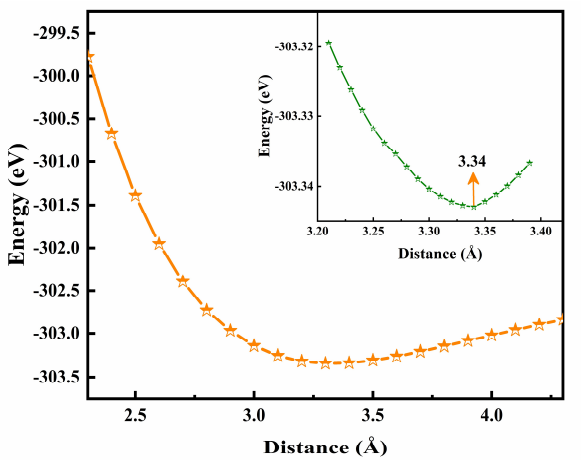

Fig. S2. Total energy as a function of the interlayer distance of borophene and MoS_2. Inset: Zooming-in near the equilibrium distance.

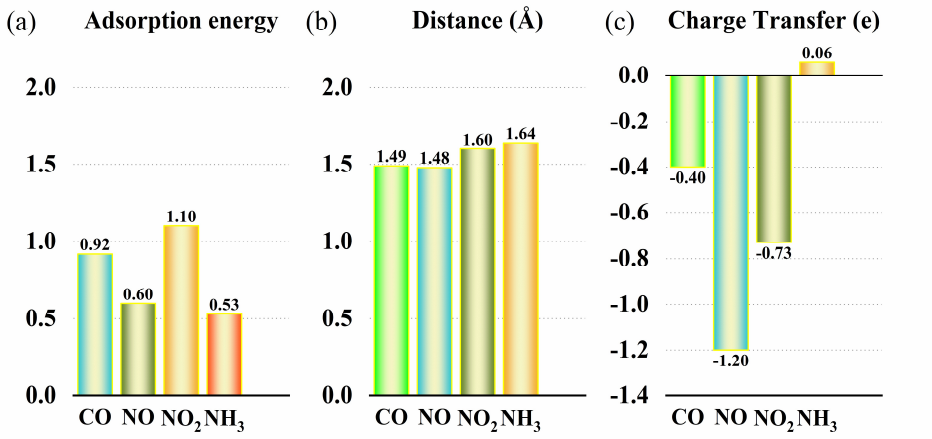

Fig.S3. Adsorption energy, shortest atomic distance between molecule and β_{12} borophene, and the charge transfer without MoS_2.

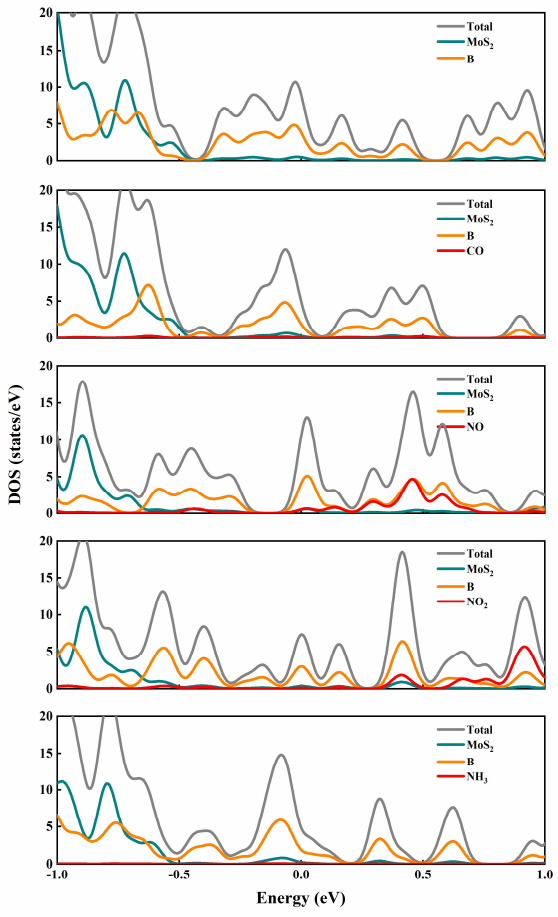

Fig. S4. Density of states of β_{12} borophene/MoS_2 structures with MoS_2. The Fermi level is shifted to zero.

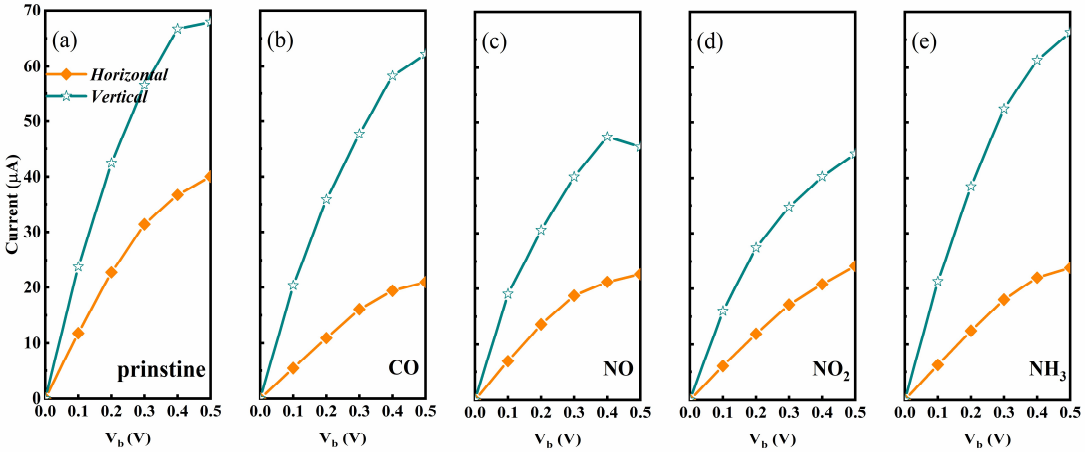

Fig. S5. Current-voltage curves of the β_{12} borophene based gas sensors with and without molecules.

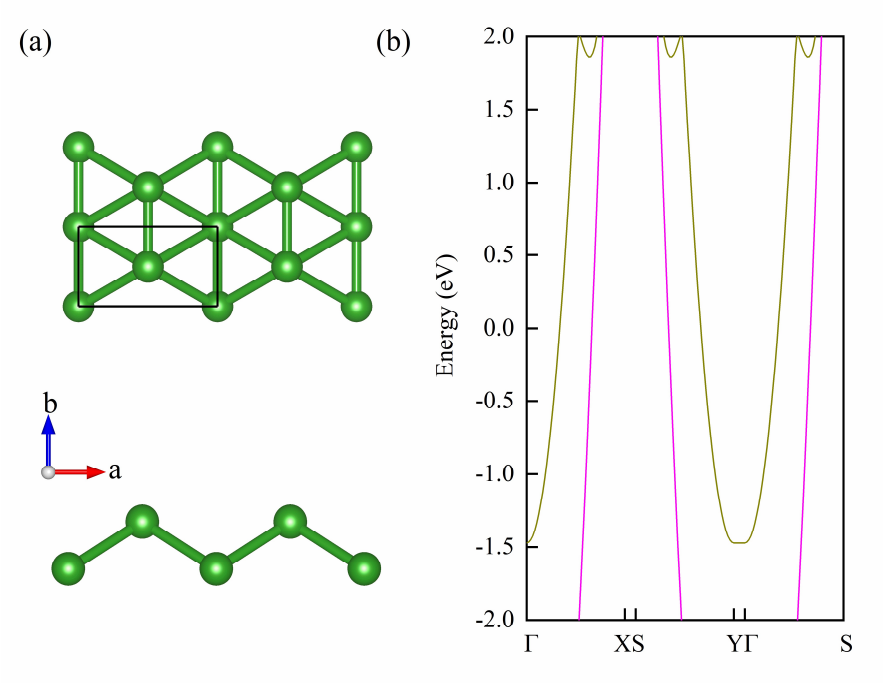

Fig. S6. Top, side view and Energy bands of buckled triangular borophene.

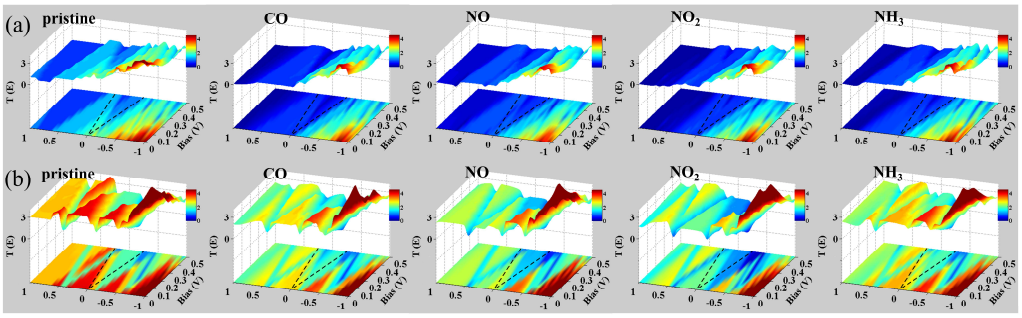

Fig. S7. Transmission spectra of pristine and CO, NO, NO_2, NH_3-adsorbed gas sensors along (a) horizontal and (b) vertical direction (3D and the related 2D projection drawing). Black dashed lines indicate the bias window and Fermi level is shifted to zero.