Frontiers of Physics
https://doi.org/10.1007/s11467-021-1094-5
Front. Phys.
17(1), 13501 (2022)

RESEARCH ARTICLE

A comprehensive first-principle study of borophene-based nano gas sensor with gold electrodes

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Received March 15, 2021; accepted June 16, 2021

SUPPLEMENTARY MATERIAL

In this supplementary material, we provide useful supporting information concerning (1) the optimized atomic details of borophene and MoS_2 heterostructure; (2) Relaxed structures of borophene monolayer after adsorption of four different gas molecules; (3) The I–V curve of ten different systems; (4) transmission for eleven different systems with or without considering the influence of gas molecules, MoS_2 substrate or gold electrodes at equilibrium state and 0.5 V bias voltage and the transmission versus moment k at Fermi energy.

1) The optimized atomic details of borophene and MoS_2 heterostructure

To construct borophene-MoS_2 heterostructure, we stretched MoS2 unite cell by 1.36% in the transport direction and 3.73% in the period direction to match borophene unite cell. To optimize the heterostructure, we chosen three highly symmetrical locations, it can be seen from Fig. S1, the boron atoms are respectively located (a, d) at the middle of the Mo and S (bridge), (b, e) above the S atom (S-Top), and (c, f) above the Mo atom (Mo-Top). After determining the three positions of the heterostructure, we calculated the energy of the three structures at different distances and plotted the energy value as a function of the distance between two materials. As shown in Fig. S1 (g), the structure Mo-Top has the lowest energy when the distance is 3.04 Å.

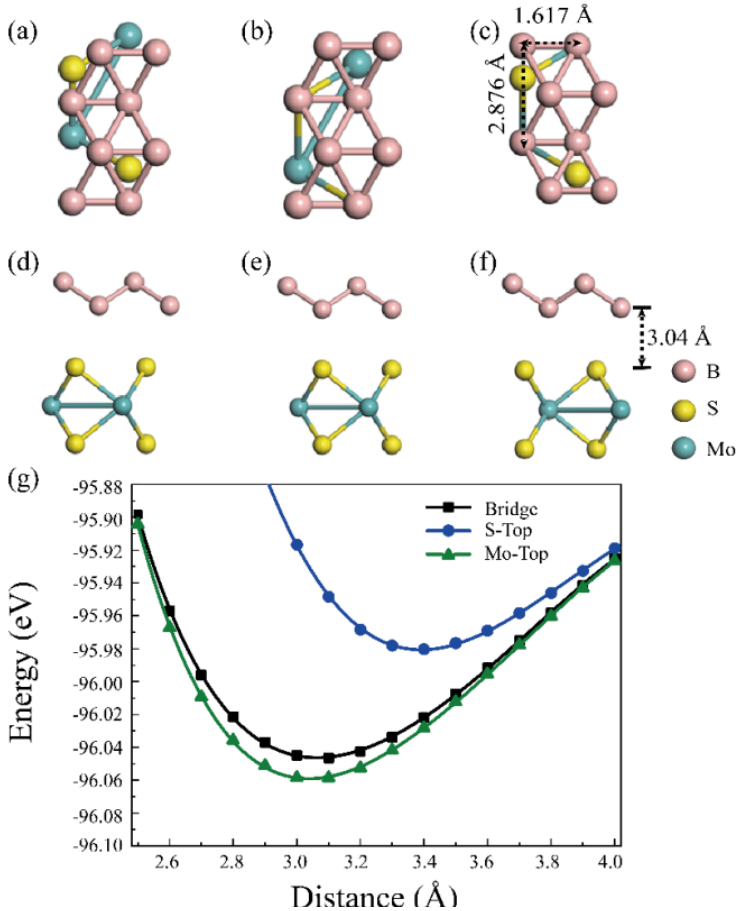

Fig. S1 (a−c) Top view and **(e−f)** side view of borophene/MOS_2 heterostructure in different stacking way. **(g)** The energy versus distance curve at three highly symmetric positions.

2) Relaxed structures of borophene monolayer after adsorption of four different gas molecules

We constructed the borophene monolayer in a 5×4 supercell as shown in Fig. S2 with lattice parameter is 6.56 Å×8.7 Å. Then we put the gas molecules on the borophene and optimize the structure in *VASP*. Pink balls represent boron atoms, while gray, red, purple and white balls represent C, O, N and H atoms, respectively. First, look at the adsorption of CO, C atom binds to the surface with a C−B distance of 1.50 Å and the angle between surface and gas (B−C−O) is 179.75°. The bond length of C-O in free-standing CO molecule is 1.14 Å, and it becomes 1.16 Å on binding with the surface. In the case of NO, the bonding distance with the surface is 1.54 Å with N−O bond length of 1.22 Å that is larger than in its isolated form (1.17 Å). Similarly, NO makes an angle of 118.4° with the surface. NO_2 is also chemisorbed on the borophene monolayer, and the shortest distance between gas and the surface is 1.58 Å. For the adsorbed NO_2, the N−O bond distance is 1.24 Å which is slightly higher than that of isolated form (1.22 Å). We find O−N−O bond angle to be 125°, which is significantly smaller than what is observed in bare NO_2 (140°). Moving on to the tetratomic gas NH_3, the shortest bonding distance from the surface is found to be 1.60 Å with N atom directly bonding with B atom of the borophene. Considering the N-H bond distance (1.03 Å) for the surface adsorbed NH_3, there is no appreciable difference from its free counterpart.

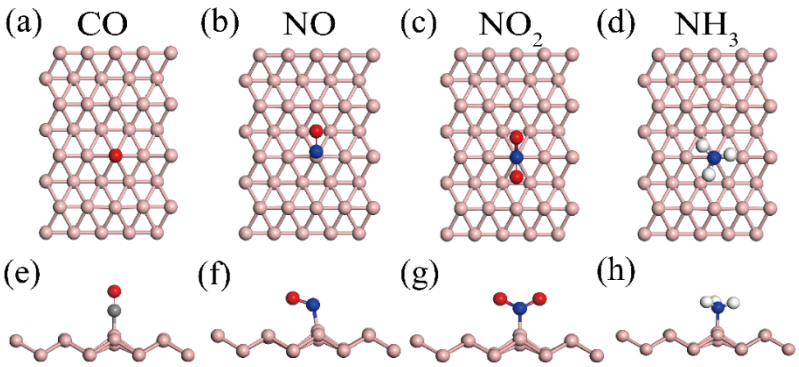

Fig. S2 The most stable configurations for **(a, e)** CO, **(b, f)** NO, **(c, g)** NO_2 and **(d, h)** NH_3 adsorbed on borophene.

3) The I-V curve of ten different systems

In Figs. S3 (a) and (b), the I-V curves of pristine borophene with and without CO molecules show linear behavior, and the red lines show their linear fitting, other I-V curves are not perfect linear. Figure S3 (c) is fitted by piecewise function. In Figs. S3 (d-j), the red lines directly connect the first and last square at 0 and 0.5 V.

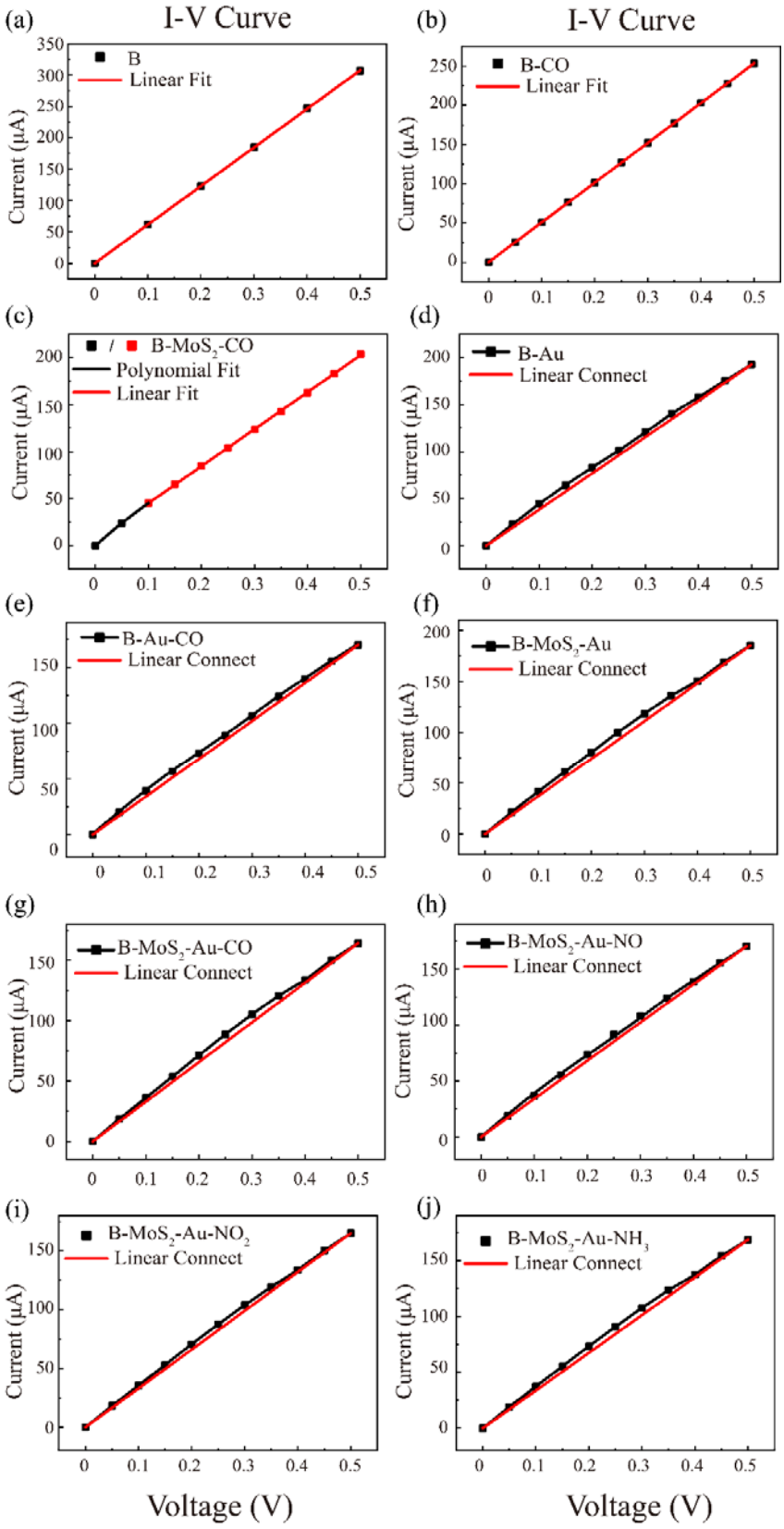

Fig. S3 *I*−*V* curves of ten different systems.

4) Transmission for eleven different systems with or without considering the influence of gas molecules, MoS2 substrate or gold electrodes at equilibrium state and 0.5 V bias voltage and the transmission versus moment k at Fermi energy

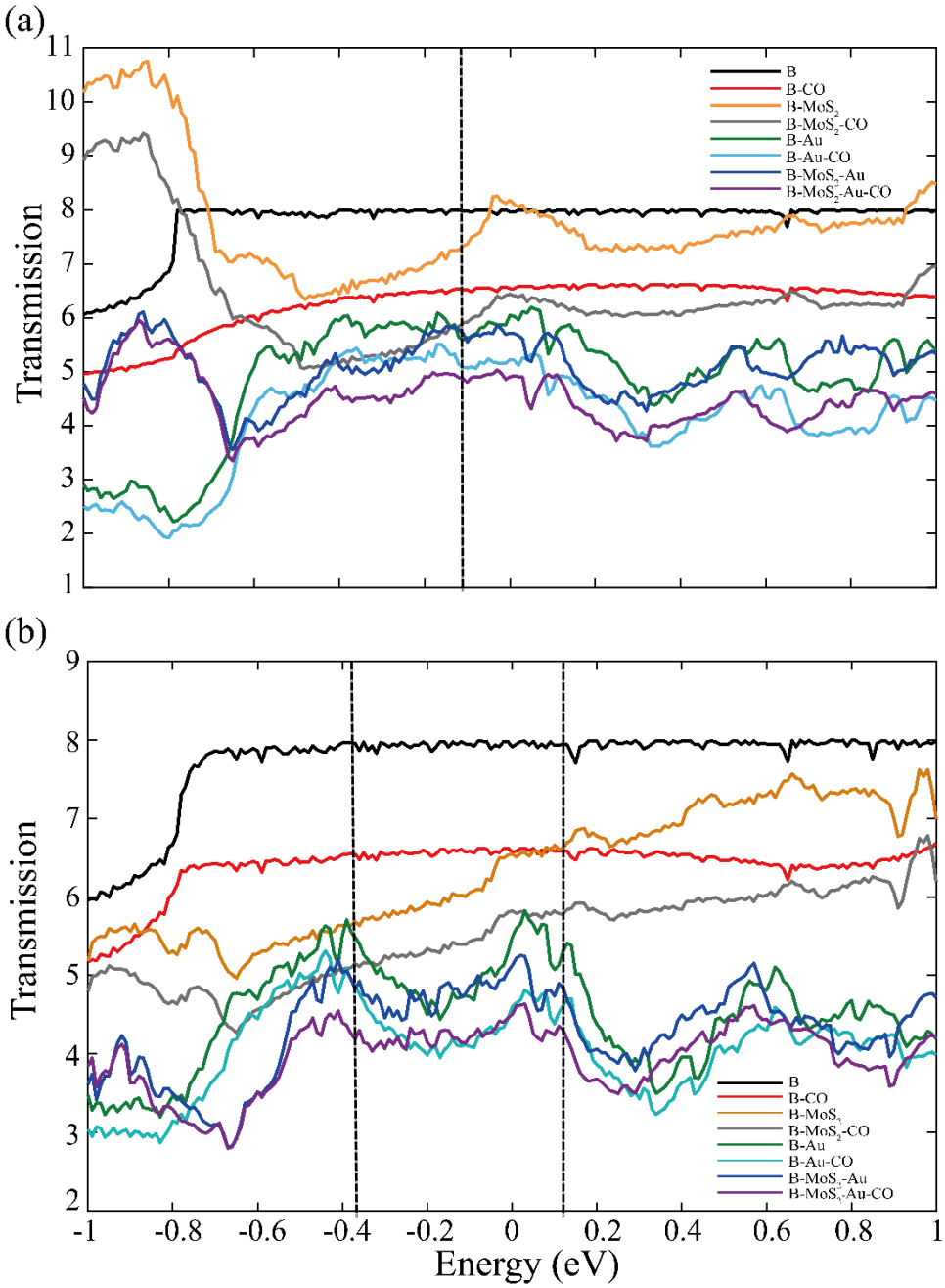

Fig. S4 Transmission versus energy **(a)** at equilibrium state and **(b)** under 0.5 V.

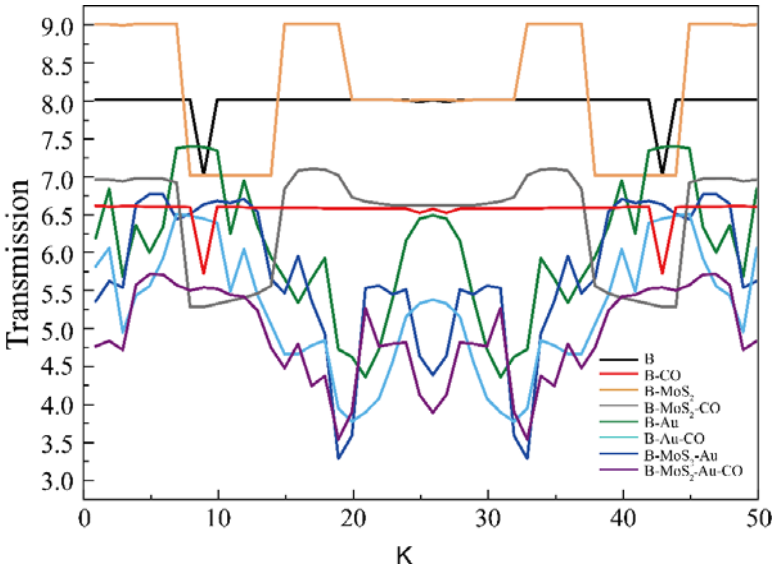

Fig. S5 Transmission versus moment k at Fermi level under 0 V.

To analyze the microscopic mechanisms of the gas sensor, the transmission spectra at $V_b = 0$ is plotted in Fig. S4(a). Under zero bias voltages, the transport properties of the gas sensor are mainly dominated by the transmission spectrum at the Fermi level. The transmission coefficients of the pure borophene gas sensor at the Fermi level is about 8, indicating that 8 transmission channels can be utilized at low bias voltages. For the B-Au gas sensor, there are about 6 transmission channels near Fermi level. Since the number of transmission channels decreases after adding gold electrodes, the current will decrease obviously. The same results can be obtained by comparing B-MoS_2 gas sensor and B-MoS_2-Au gas sensor. Non-equilibrium transmission at 0.5 V in Fig. S4(b) and transmission versus moment k curve in Fig. S5 both support the analysis.