Supplementary Information

Gas sensing properties of buckled bismuthene predicted by first-principles calculation

Wenfeng Pan,† Ning Qi,*† Bin Zhao,‡ Sheng Chang,† Shizhuo Ye,† and Zhiquan Chen*†

†Hubei Nuclear Solid Physics Key Laboratory, Department of Physics, Wuhan University, Wuhan 430072, China
‡College of Science, Zhongyuan University of Technology, Zhengzhou 450007, China
E-mail: ningqi@whu.edu.cn; chenzq@whu.edu.cn

Contents:

Fig. S1: The total (DOS) and partial (PDOS) electronic density of states for (a) pristine b-Bi and b-Bi adsorbed with (b) CO, (c) O₂, (d) H₂O, (e) NH₃, (f) SO₂, (g) NO, (h) NO₂ (with SOC).

Fig. S2: The I – V curves along the zigzag and armchair direction of pristine b-Bi and b-Bi with NH₃ adsorption.

Fig. S3: Diffusion energy barrier of (a) NH₃, (b) O₂, (c) NO and (d) NO₂ on b-Bi along armchair and zigzag directions.
Fig. S1: The total (DOS) and partial (PDOS) electronic density of states for (a) pristine $b$-Bi and $b$-Bi adsorbed with (b) CO, (c) O$_2$, (d) H$_2$O, (e) NH$_3$, (f) SO$_2$, (g) NO, (h) NO$_2$ (with SOC). The Fermi level is set to zero and indicated by the black dashed line.
Fig. S2: The $I - V$ curves along the zigzag and armchair direction of pristine $b$-Bi and $b$-Bi with NH$_3$ adsorption.
Fig. S3: Diffusion energy barrier of (a) NH$_3$, (b) O$_2$, (c) NO and (d) NO$_2$ on b-Bi along armchair and zigzag directions. The configurations of initial state (IS), transition states along armchair direction (TS$_A$) and along the zigzag direction (TS$_Z$), final states along armchair direction (FS$_A$) and along zigzag direction (FS$_Z$) are included in the figure.