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

Supplementary Information

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

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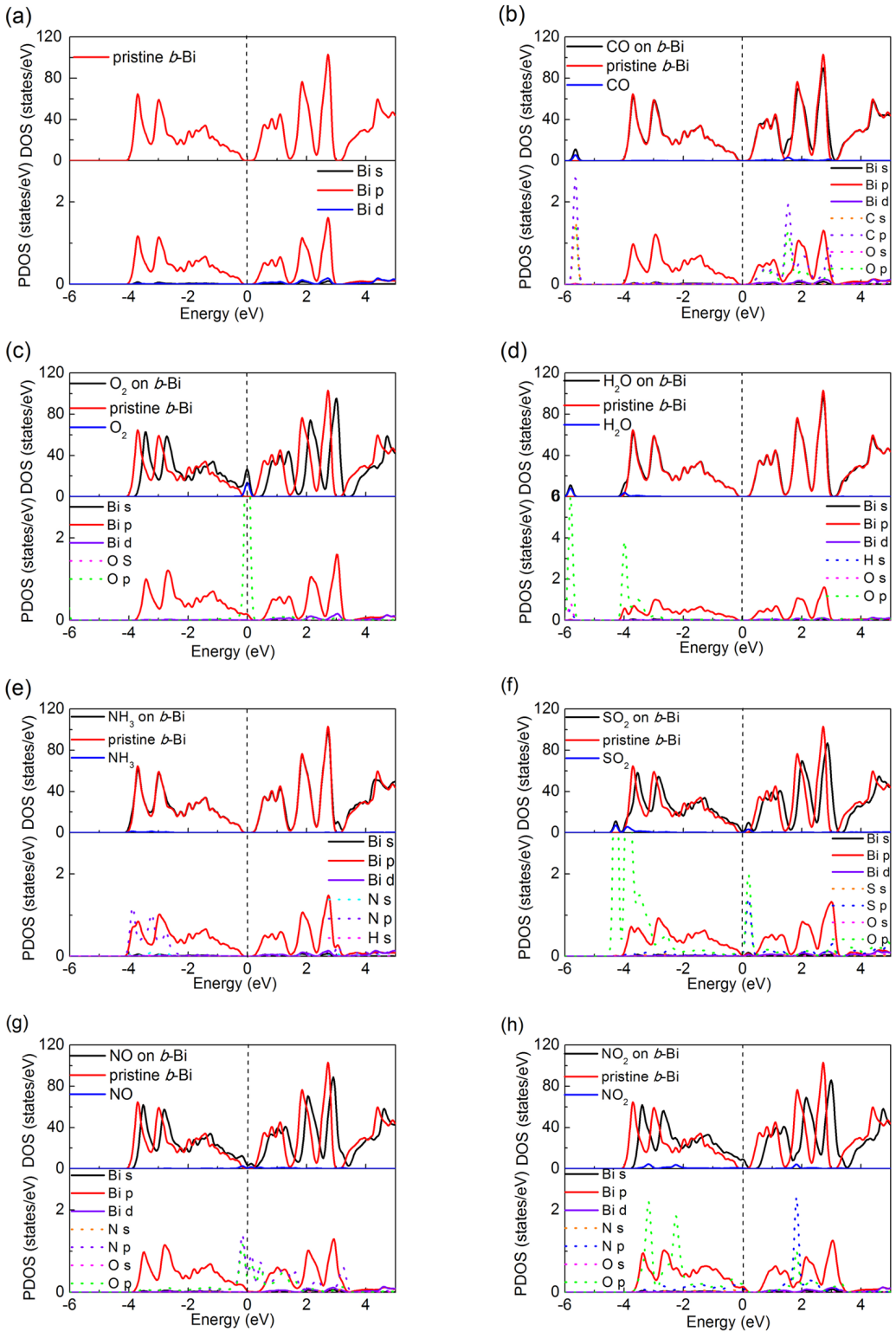

Fig. S1: The total (DOS) and partial (PDOS) electronic density of states for (a) pristine *b*-Bi and *b*-Bi adsorbed with (b) CO, (c) O_2, (d) H_2O, (e) NH_3, (f) SO_2, (g) NO, (h) NO_2 (with SOC). The Fermi level is set to zero and indicated by the black dashed line.

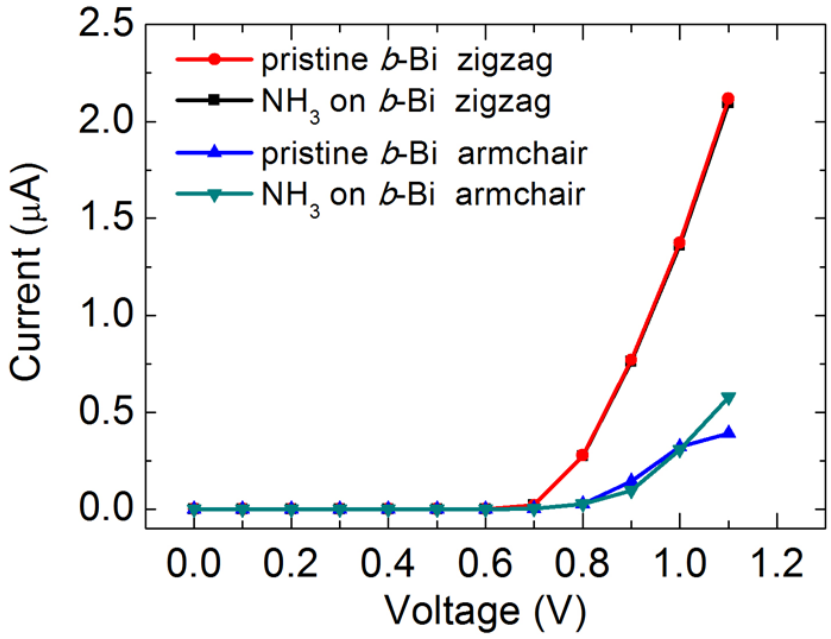

Fig. S2: The $I-V$ curves along the zigzag and armchair direction of pristine b-Bi and b-Bi with NH_3 adsorption.

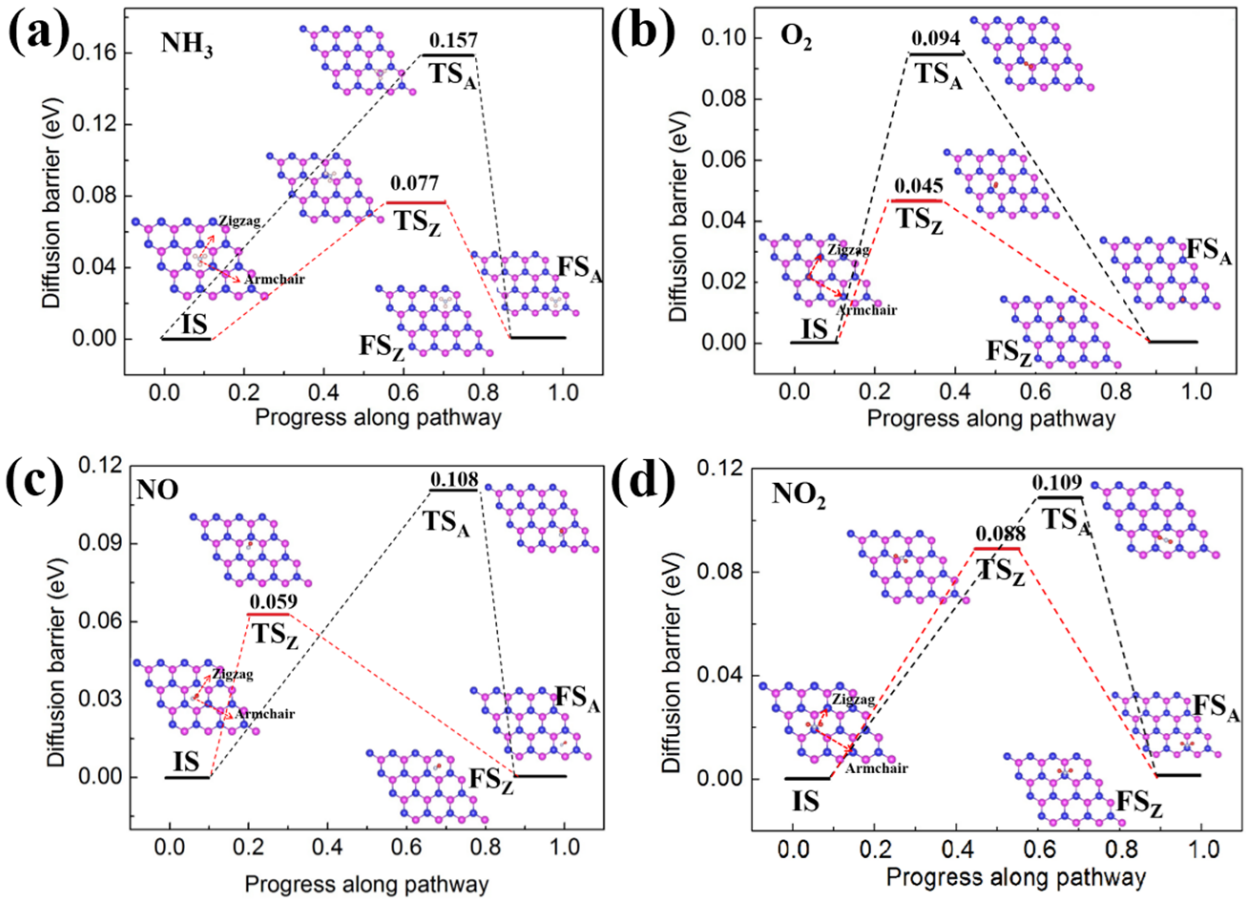

Fig. S3: Diffusion energy barrier of (a) NH_3, (b) O_2, (c) NO and (d) NO_2 on *b*-Bi along armchair and zigzag directions. The configurations of initial state (IS), transition states along armchair direction (TS_A) and along the zigzag direction (TS_Z), final states along armchair direction (FS_A) and along zigzag direction (FS_Z) are included in the figure.