Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Toxic Gas Sensing Performance of Arsenene functionalized by Single-atom (Ag, Au): a DFT Study

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Table S1 Total energy (E_t) of NO/Ag-arsenene after fully relaxation with various K-points in supercell of (4×4×1).

K-points	5×5×1	7×7×1	9×9×1
E_t (eV)	-163.3871	-163.3862	-163.3859

Table S2 Total energy (E_t) of NO/Ag-arsenene after fully relaxation with various energy cutoff.

$E_{cut\text{-}off}$(eV)	400	420	450	500
E_t (eV)	-163.3891	-163.3871	-163.3862	-163.3894

Table S3 Total energy (E_t) for NO/Ag-arsenene system with different vacuum height.

vacuum height(Å)	20	22	25
E_t (eV)	-163.3862	-163.3865	-163.3862

Table S4 Adsorption energy (E_{ads}) for NO adsorbed on Ag-arsenene surface with different size of supercell.

supercell	4×4×1	5×5×1	6×6×1
E_{ads} (eV)	-0.724	-0.726	-0.727

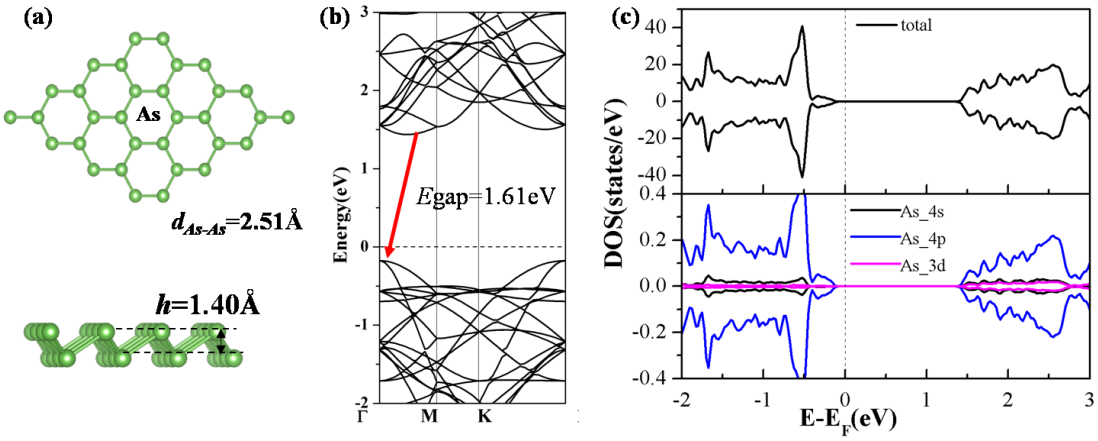

Figure S1 (a)-(c) Optimized structures, band structure and density of states (PDOS) for pristine arsenene, respectively.

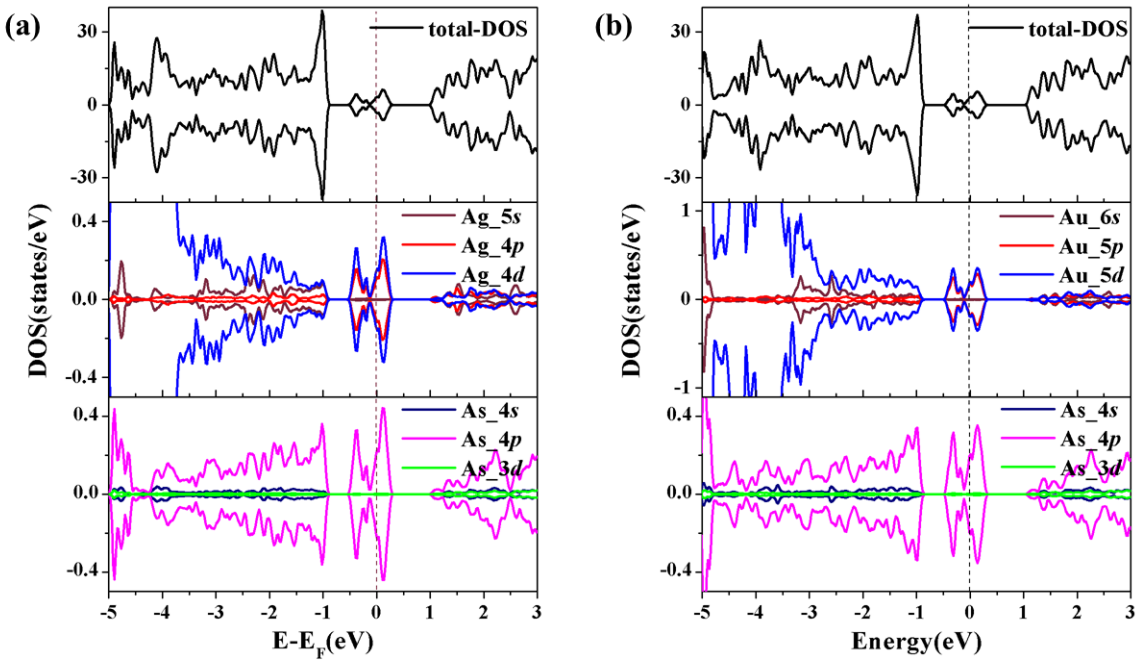

Figure S2 (a)-(b) Total density of states (TDOS) and Project Density of states (PDOS) for Ag and Au-doped arsenene systems, respectively.

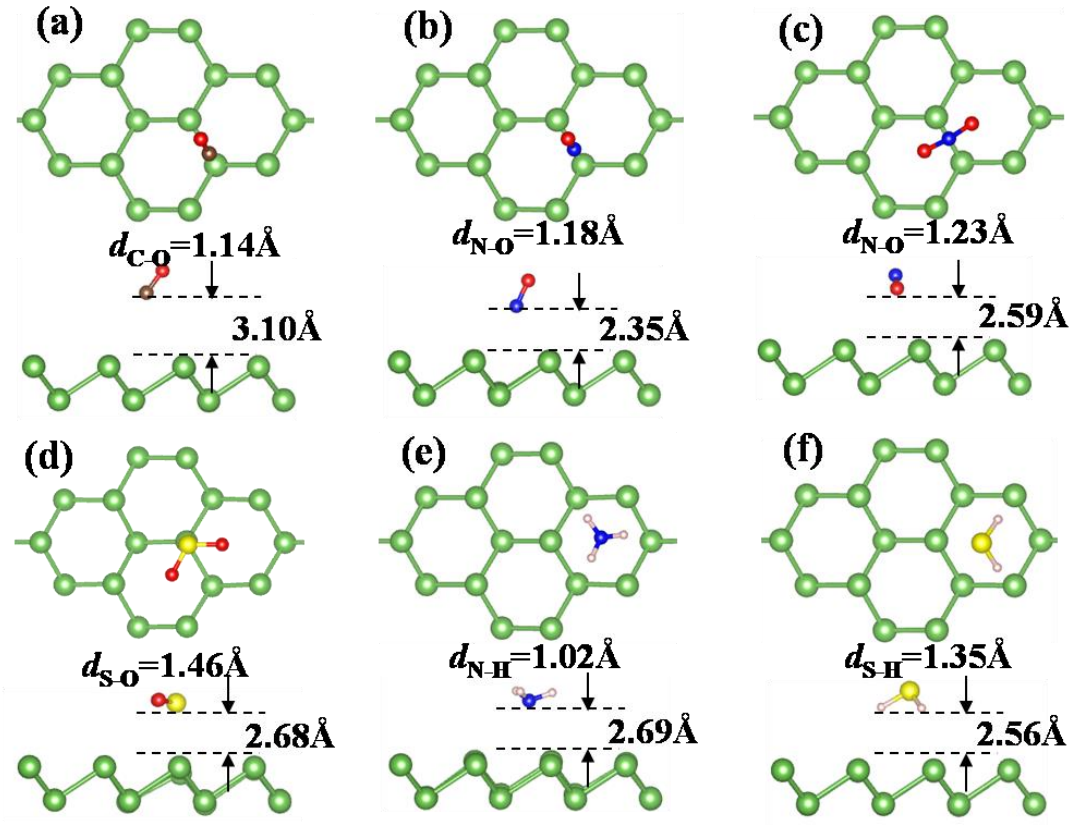

Figure S3 (a)-(f) Top (upper panel) and side views (lower panel) of the most favorable configurations of pristine arsenene with adsorption of CO, NO, NO_2, SO_2, NH_3 and H_2S, respectively.

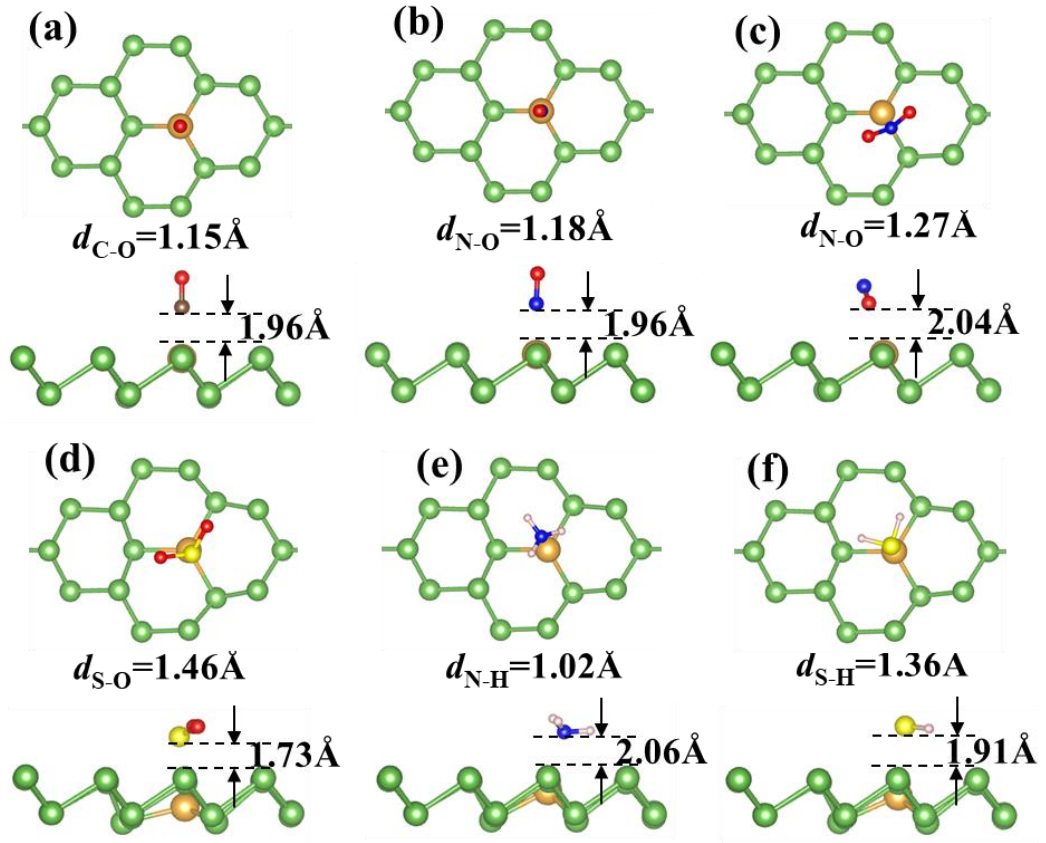

Figure S4 (a)-(f) Top (upper panel) and side views (lower panel) of the most favorable configurations of Au-arsenene with the adsorption of CO, NO, NO_2, SO_2, NH_3 and H_2S, respectively.

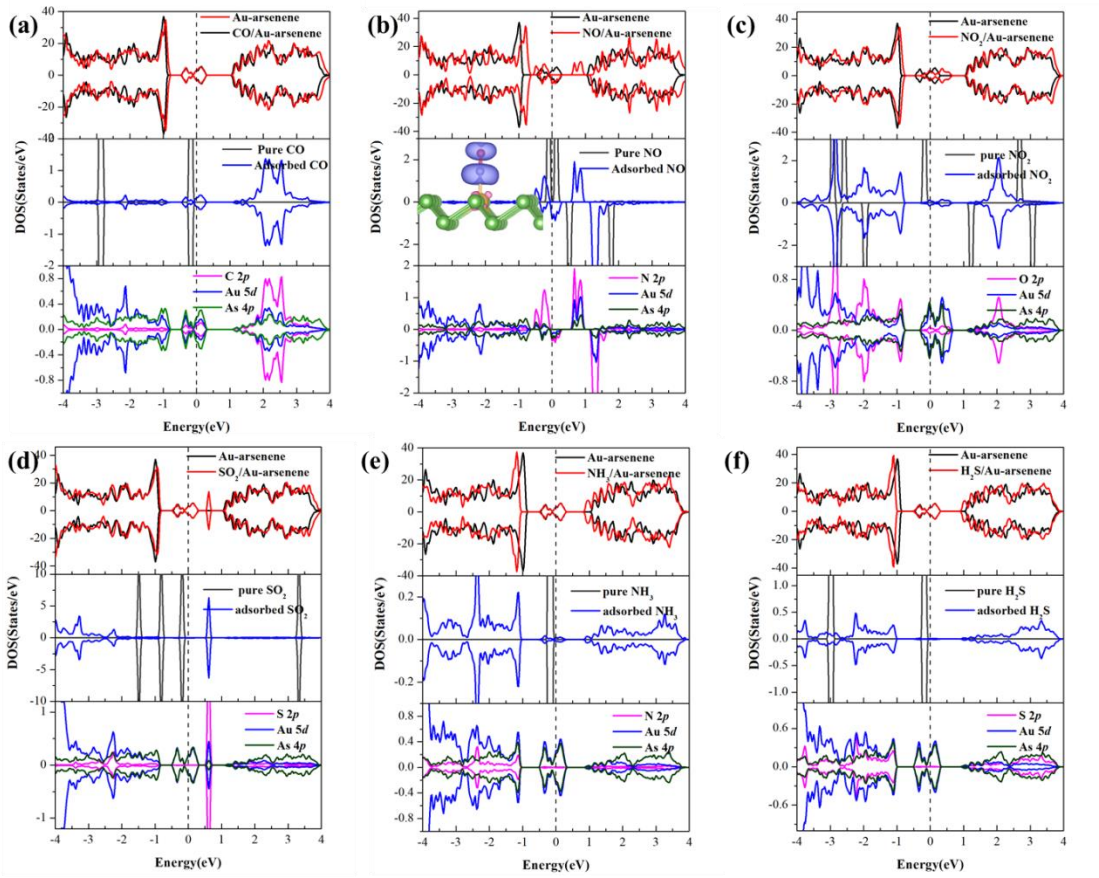

Figure S5 (a)-(f) Density of states (PDOS) for considered gas molecules CO, NO, NO_2, SO_2, NH_3 and H_2S adsorbed at Au-arsenene, respectively. E_F is set to be 0 eV denoted by dash lines. The magnetization charge density difference for NO/Au-arsenene is plotted in the insert of (b) and the magnetization charge density isosurface value is 0.001e/Å^3.

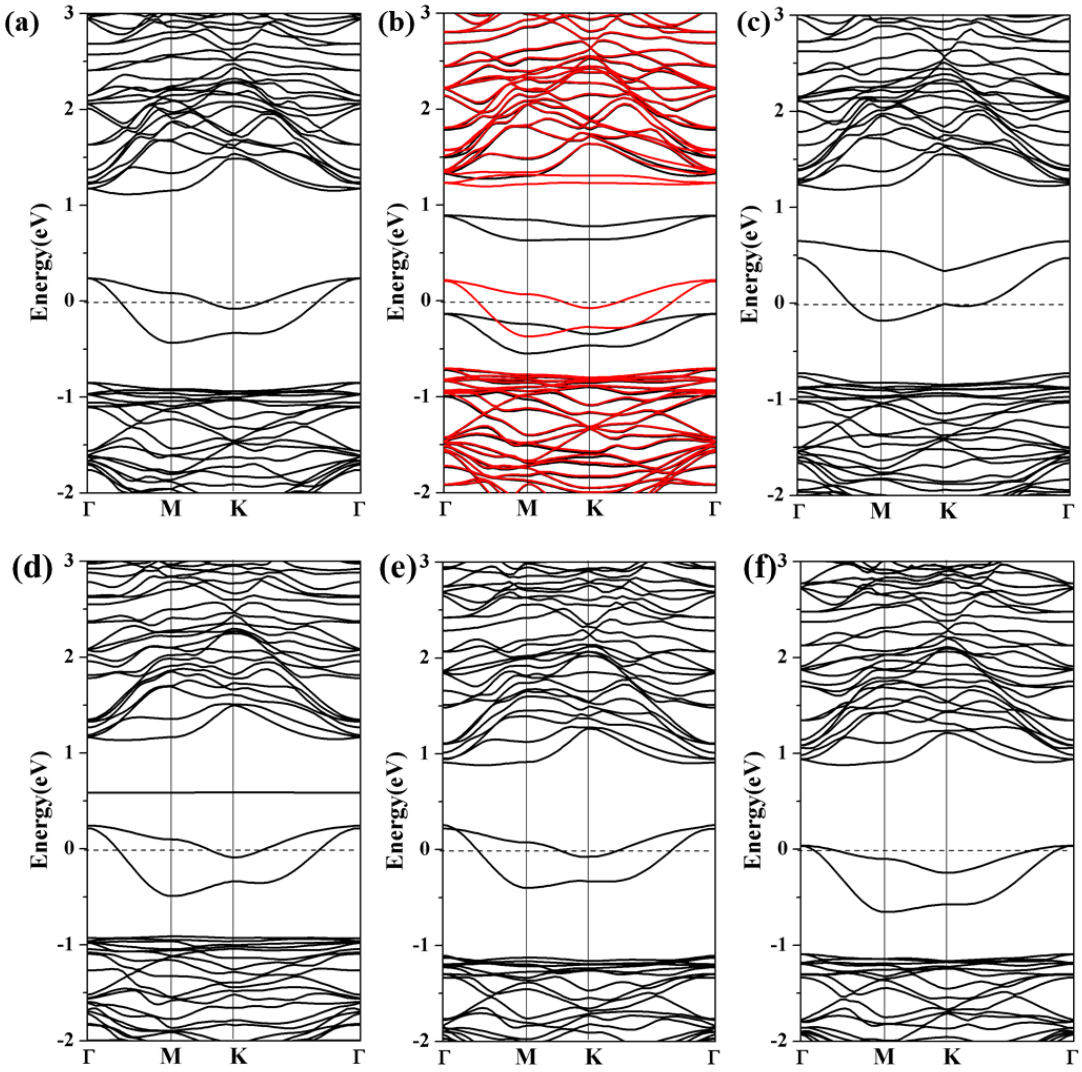

Figure S6 (a)-(f) Spin-polarized band structures for CO, NO, NO_2, SO_2, NH_3 and H_2S adsorbed at Au-arsenene, respectively. The black and red lines show spin up and spin down band structures, respectively. E_F is set to be 0eV denoted by the black dash lines.

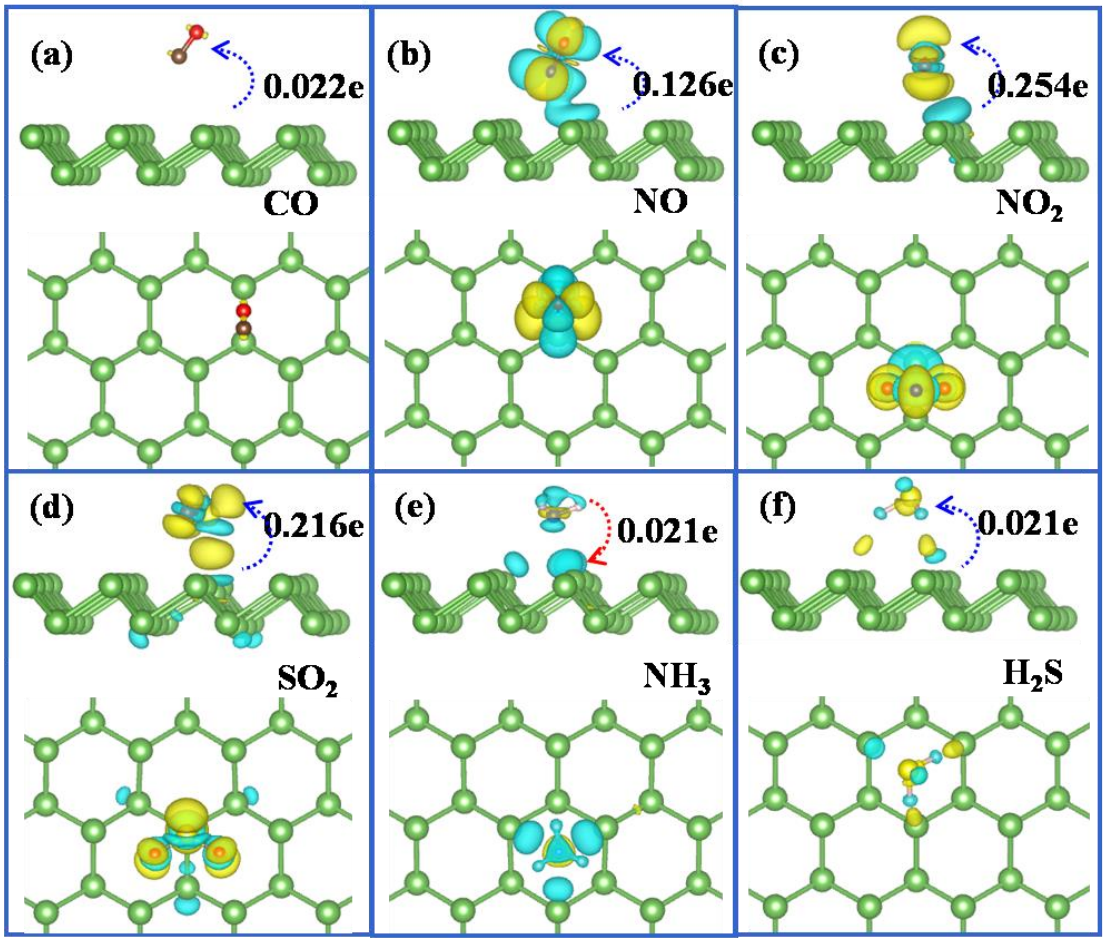

Figure S7 (a)-(f) Top (upper panel) and side views (lower panel) of the charge density difference for the most favorable configurations of pristine arsenene with adsorption of CO, NO, NO_2, SO_2, NH_3 and H_2S, respectively.