Supporting Information

Janus MoSSe monolayer: superior and strain-sensitive gas sensing material

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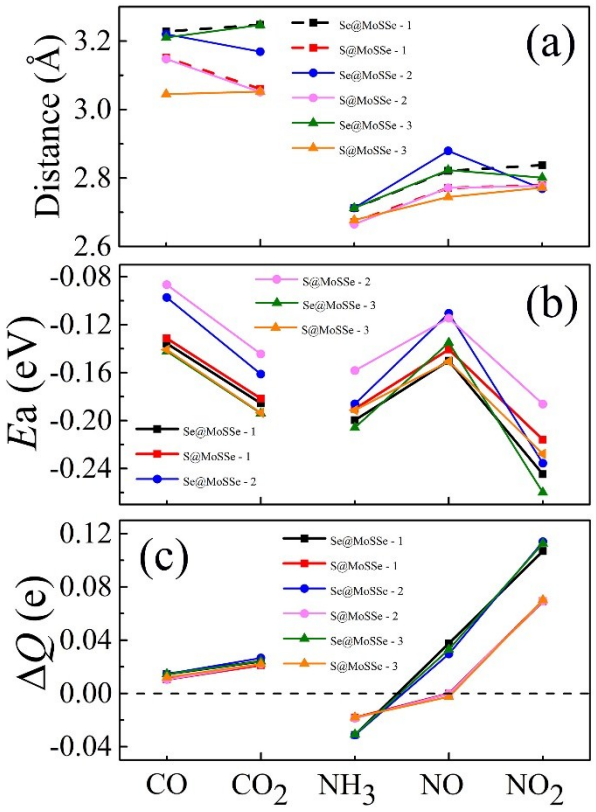

Fig. S1 The value of (a) adsorption distance d (Å), (b) adsorption energy E_a (eV), and (c) charge transfer ΔQ (e) of gas molecules CO, CO_2, NH_3, NO and NO_2 adsorption on Se-layer, S-layer, respectively with different vdW correction methods (Method 1: the

zero damping DFT-D3 method of Grimme, which we adopt in this paper; Method 2: the DFT-D2 method of Grimme; Method 3: the DFT-D3 method with Becke-Jonson damping). The positive (negative) value of charge transfer represents gaining (losing) charge of the adsorbed gas molecule from (to) the layer.

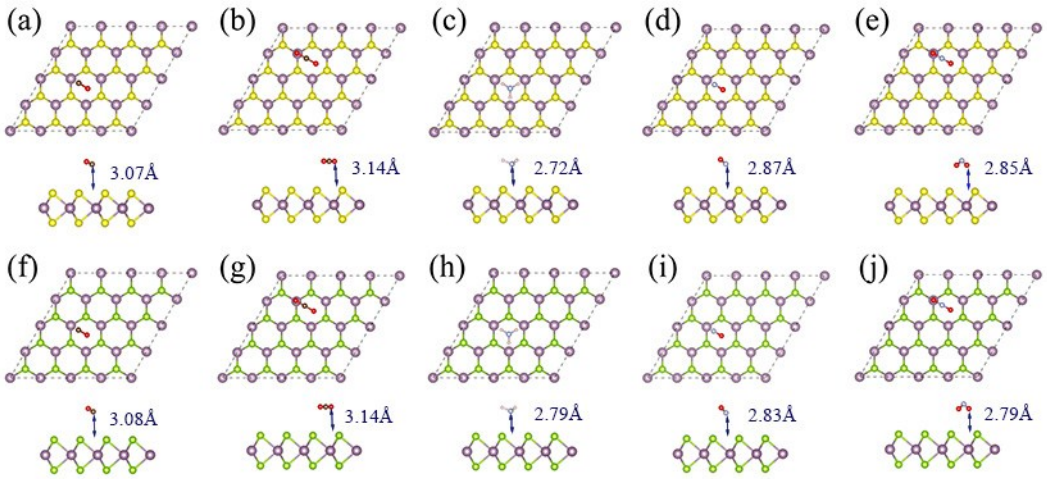

Fig. S2 Structural models and optimized structures of gas molecules CO, CO_2, NH_3, NO and NO_2 adsorption on the MoS_2 (a-e) and $MoSe_2$ (f-j). The atoms of monolayer and adsorbed molecules are denoted. The 4×4 super cell of MoS_2 ($MoSe_2$) monolayer is represented by the dashed lines. Purple, green and yellow balls are Mo, Se and S atoms respectively. Black, red, light grey and light pink represent C, O, N and H atoms respectively.

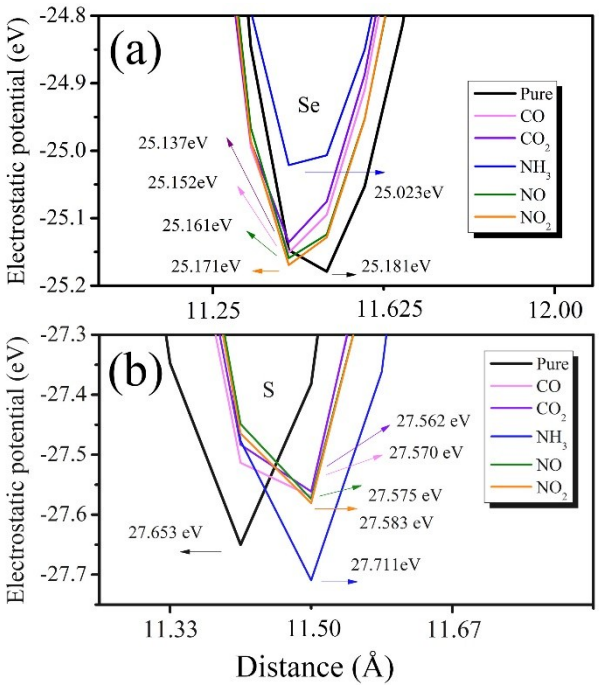

Fig. S3 The variation of electrostatic potential Φ (eV) of (a) Se surface, and (b) S surface of the gas molecule CO, CO_2, NH_3, NO and NO_2 adsorption on Se-layer (S-layer), in comparison to pure Janus MoSeS structure. The corresponding electrostatic potential values are denoted with the different colors.

Tab. S1 Calculated the electrostatic potential shifting values $\Delta\Phi$ (eV) of Se (S) surface of the gas molecule CO, CO_2, NH_3, NO and NO_2 adsorption on Se-layer (S-layer), in comparison to pure Janus MoSeS structure. The positive (negative) value of $\Delta\Phi$ represents up-shifting (down-shifting) of the gas molecule adsorbed surface.

$\Delta\Phi$ (eV)	CO	CO_2	NH_3	NO	NO_2
Se-layer	0.03	0.04	0.16	0.02	0.01
S-layer	0.08	0.09	-0.06	0.08	0.07

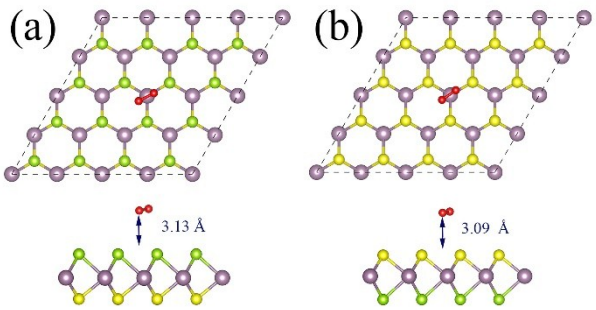

Fig. S4 Structural models and optimized structures of gas molecule O_2 adsorption on the (a) Se-layer, and (b) S-layer. The atoms of monolayer and adsorbed molecules are denoted. The 4×4 super cell of Janus MoSSe monolayer is represented by the dashed lines. Purple, green, yellow and red balls are Mo, Se, S and O atoms respectively.

Tab. S2 Calculated adsorption distance d (Å), adsorption energy E_a (eV), and charge transfer ΔQ (e) of gas molecule O_2 adsorption on Se-layer, S-layer, respectively. The positive value of charge transfer represents gaining charge of the adsorbed gas molecule from the layer.

Adsorption surface	d (Å)	E_a (eV)	ΔQ(e)
Se-layer	3.13	-0.104	0.035
S-layer	3.09	-0.101	0.018

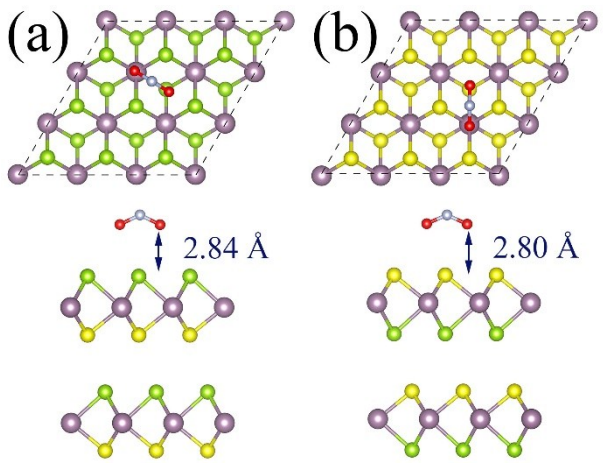

Fig. S5 Structural models and optimized structures of gas molecule NO_2 adsorption on the (a) Se-bi-layer, and (b) S-bi-layer. The atoms of monolayer and adsorbed molecules are denoted. The 3×3 super cell of Janus MoSSe monolayer is represented by the dashed lines. Purple, green, yellow, light grey and red balls are Mo, Se, S, N and O atoms respectively.

Tab. S3 Calculated adsorption distance d (Å), adsorption energy E_a (eV), and charge transfer ΔQ (e) of gas molecule NO_2 adsorption on Se-layer, Se-bi-layer, S-layer, and S-bi-layer, respectively. The positive value of charge transfer represents gaining charge of the adsorbed gas molecule from the layer.

Adsorption surface	d (Å)	E_a (eV)	ΔQ(e)
Se-layer	2.84	-0.245	0.107
Se-bi-layer	2.84	-0.312	0.186
S-layer	2.78	-0.216	0.069
S-bi-layer	2.80	-0.222	0.072

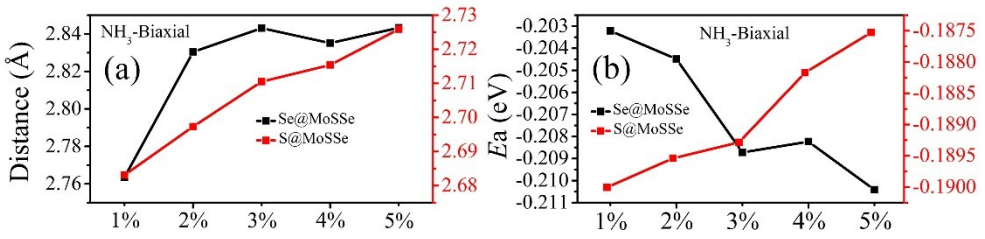

Fig. S6 The variation of (a) adsorption distance *d* (Å), and (b) adsorption energy E_a (eV) of the gas molecule NH_3 adsorption on Se-layer and S-layer, respectively, as the function of applied biaxial tensile strain.

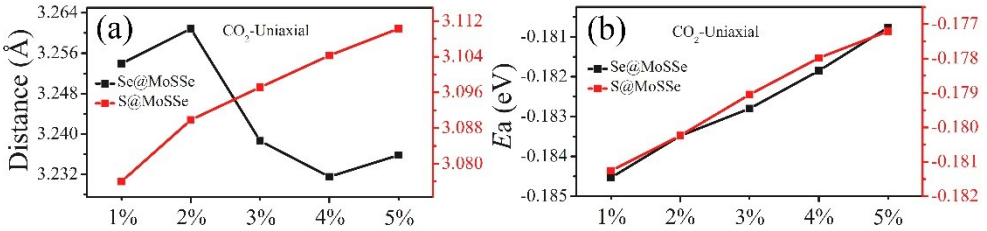

Fig. S7 The variation of (a) adsorption distance *d* (Å), and (b) adsorption energy E_a (eV) of the gas molecule CO_2 adsorption on Se-layer and S-layer, respectively, as the function of applied uniaxial tensile strain.