Supplementary Materials

Sensing the polar molecules MH_3 (M=N, P, or As) with Janus NbTeSe monolayer

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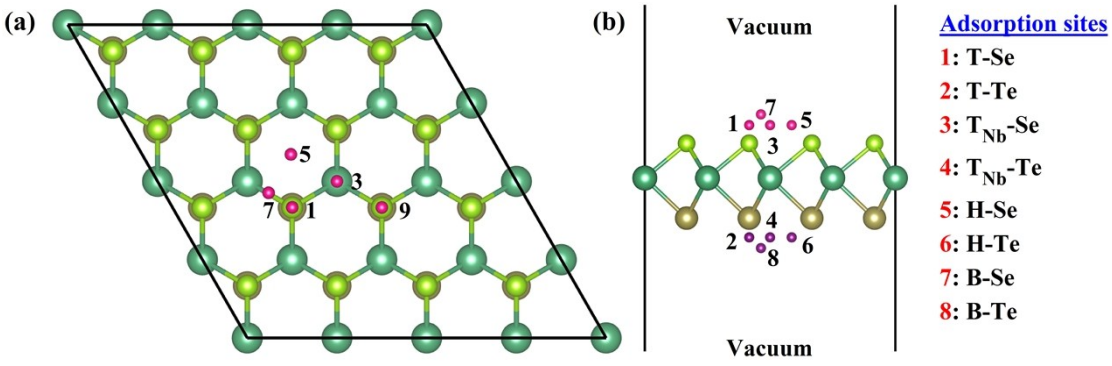

Figure S1. The structure of Janus NbSeTe monolayer from (a) top and (b) side views with possible adsorption positions for molecule NH_3, PH_3 and AsH_3, respectively.

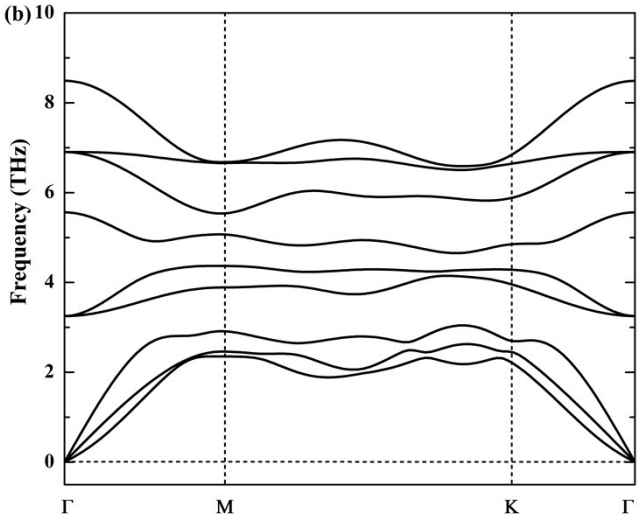

Figure S2. Calculated phonon band dispersion of Janus NbSeTe monolayer.

Table S1. The bond lengths and angles for NH_3, PH_3 and AsH_3 gas molecules before and after adsorbed on Janus NbTeSe monolayer, respectively, corresponding to the adsorption energies in Figure S1.

Type		Bond length of the molecule (Å)			Angle of the molecule (°)		
		NH_3	PH_3	AsH_3	NH_3	PH_3	AsH_3
Pristine		1.028	1.433	1.539	106.046	92.328	90.911
Upward orientation	T-Se	1.027	1.434	1.541	106.906	92.559	91.218
	T-Te	1.028	1.433	1.541	105.726	91.851	90.621
	T_{Nb}-Se	1.028	1.434	1.541	106.375	92.303	90.828
	T_{Nb}-Te	1.028	1.434	1.540	106.132	92.058	90.659
	H-Se	1.027	1.432	1.541	106.806	92.486	91.078
	H-Te	1.028	1.434	1.540	106.252	92.058	90.659
	B-Se	1.027	1.433	1.540	106.655	92.535	91.239
	B-Te	1.028	1.433	1.541	105.924	91.927	90.628
Downward orientation	T-Se	1.025	1.432	1.540	106.516	93.170	91.400
	T-Te	1.029	1.421	1.525	106.693	93.059	91.358
	T_{Nb}-Se	1.027	1.431	1.540	106.754	93.021	91.373
	T_{Nb}-Te	1.027	1.432	1.540	106.804	92.939	91.277
	H-Se	1.026	1.431	1.540	107.335	93.092	92.128
	H-Te	1.027	1.432	1.541	107.264	93.656	91.967
	B-Se	1.026	1.431	1.540	107.655	93.014	91.235
	B-Te	1.018	1.432	1.540	106.335	92.753	91.394

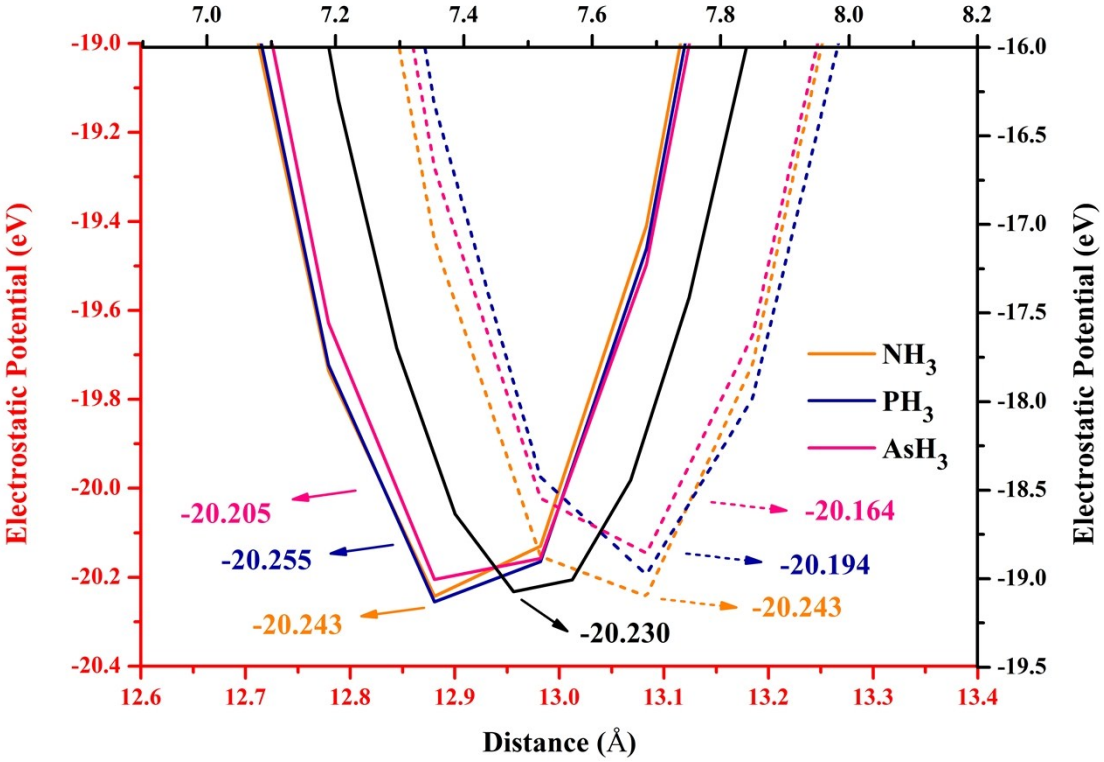

Figure S3. The electrostatic potential ϕ (eV) of Se surface (solid lines) and Te (dash lines) surface of the gas molecule NH_3, PH_3 and AsH_3 adsorption on Se-layer and Te-layer. In comparison to pure Janus NbTeSe monolayer. The corresponding electrostatic potential values are denoted with the different colors.

Table S2. Calculated the electrostatic potential shifting values Δϕ (eV) of Se and Te surfaces of the gas molecule NH_3, PH_3 and AsH_3 adsorption on Te-layer (Se-layer), in comparison to pure Janus NbTeSe monolayer. The positive (negative) value of Δϕ represents up-shifting (down-shifting) of the gas molecule adsorbed surface, respectively.

Δϕ	NH_3	PH_3	AsH_3
Se-layer	-0.025	-0.013	0.025
Te-layer	-0.013	0.036	0.066

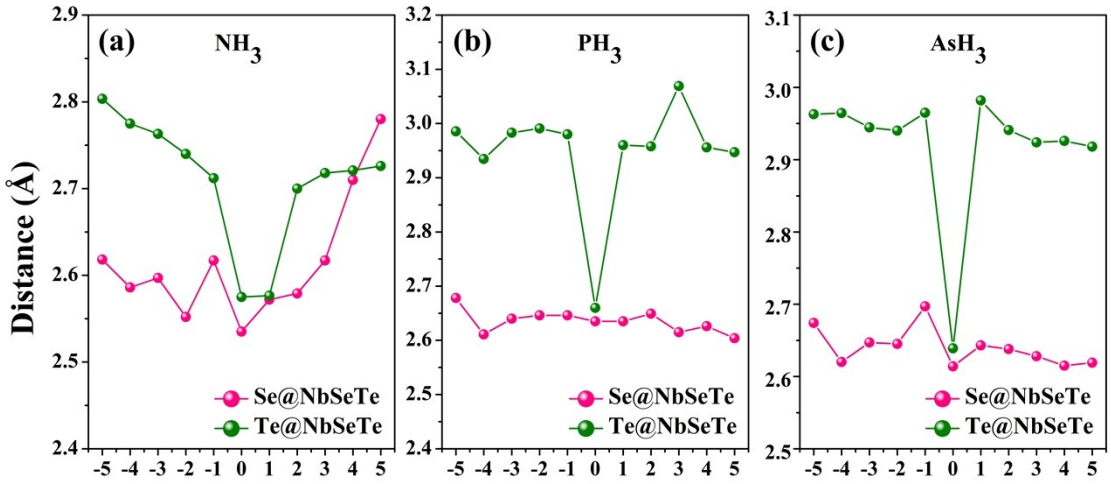

Figure S4. The variation of adsorption distance for NH_3, PH_3 and AsH_3 adsorbed on Se-layer and Te-layer, respectively, as the function of applied biaxial tensile strain.