Electronic Supplementary Information:

Effects of External Electric Field on the Sensing Property of Volatile Organic Compounds over Janus MoSSe Monolayer: A First-principles Investigation

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Table S1. Summary of the orientations for the positive external electric fields ($\vec{F}$), acetone molecule, and TMDs monolayers with their corresponding adsorption energy, E_{ads}, in different adsorption structures of acetone on pristine MoS_2 and Janus MoSSe monolayers.

E-field	Adsorption type	MoS_2				MoSSe-S				MoSSe-Se			
		$\vec{F}$	Acetone	Surface	E_{ads} (eV)	$\vec{F}$	Acetone	Surface	E_{ads} (eV)	$\vec{F}$	Acetone	Surface	E_{ads} (eV)
0.6	Ace_{v1}	↑	↓	No	0.28	↑	↓	↑	-0.05	↑	↓	↓	0.57
0.6	Ace_{v2}	↑	↑	No	-0.49	↑	↑	↑	-0.85	↑	↑	↓	0.21
0.6	Ace_{h}	↑	←	No	-0.17	↑	←	↑	-0.50	↑	←	↓	-0.11
0.4	Ace_{v1}	↑	↓	No	0.02	↑	↓	↑	-0.20	↑	↓	↓	0.26
0.4	Ace_{v2}	↑	↑	No	-0.52	↑	↑	↑	-0.77	↑	↑	↓	-0.10
0.4	Ace_{h}	↑	←	No	-0.31	↑	←	↑	-0.55	↑	←	↓	-0.26
0.2	Ace_{v1}	↑	↓	No	-0.11	↑	↓	↑	-0.21	↑	↓	↓	0.02
0.2	Ace_{v2}	↑	↑	No	-0.40	↑	↑	↑	-0.53	↑	↑	↓	-0.20
0.2	Ace_{h}	↑	←	No	-0.34	↑	←	↑	-0.42	↑	←	↓	-0.26
0	Ace_{v1}	No	↓	No	-0.24	No	↓	↑	-0.22	No	↓	↓	-0.22
0	Ace_{v2}	No	↑	No	-0.29	No	↑	↑	-0.29	No	↑	↓	-0.29
0	Ace_{h}	No	←	No	-0.36	No	←	↑	-0.32	No	←	↓	-0.32

Table S2. Summary of the orientations for the negative external electric fields ($\vec{F}$), acetone molecule, and TMDs monolayers with their corresponding adsorption energy, E_{ads}, in different adsorption structures of acetone on pristine MoS_2 and Janus MoSSe monolayers.

		MoS_2				MoSSe-S				MoSSe-Se			
E-field	Adsorption type	$\vec{F}$	Acetone	Surface	E_{ads} (eV)	$\vec{F}$	Acetone	Surface	E_{ads} (eV)	$\vec{F}$	Acetone	Surface	E_{ads} (eV)
-0.6	Ace_{v1}	↓	↓	No	-0.50	↓	↓	↑	-0.11	↓	↓	↓	-0.84
-0.6	Ace_{v2}	↓	↑	No	0.18	↓	↑	↑	0.51	↓	↑	↓	-0.13
-0.6	Ace_{h}	↓	←	No	-0.36	↓	←	↑	0.03	↓	←	↓	-0.65
-0.4	Ace_{v1}	↓	↓	No	-0.52	↓	↓	↑	-0.25	↓	↓	↓	-0.74
-0.4	Ace_{v2}	↓	↑	No	-0.06	↓	↑	↑	0.17	↓	↑	↓	-0.27
-0.4	Ace_{h}	↓	←	No	-0.44	↓	←	↑	-0.19	↓	←	↓	-0.66
-0.2	Ace_{v1}	↓	↓	No	-0.39	↓	↓	↑	-0.23	↓	↓	↓	-0.48
-0.2	Ace_{v2}	↓	↑	No	-0.17	↓	↑	↑	-0.05	↓	↑	↓	-0.26
-0.2	Ace_{h}	↓	←	No	-0.38	↓	←	↑	-0.24	↓	←	↓	-0.50
0	Ace_{v1}	No	↓	No	-0.24	No	↓	↑	-0.22	No	↓	↓	-0.22
0	Ace_{v2}	No	↑	No	-0.29	No	↑	↑	-0.29	No	↑	↓	-0.29
0	Ace_{h}	No	←	No	-0.36	No	←	↑	-0.32	No	←	↓	-0.32

Table S3. Summary of the orientations for the external electric fields ($\vec{F}$), cyclohexane molecule, and TMDs monolayers with their corresponding adsorption energy, E_{ads}, in the adsorption of cyclohexane on pristine MoS_2 and Janus MoSSe monolayers.

	MoS_2				MoSSe-S				MoSSe-Se			
E-field	$\vec{F}$	Cyclohexane	Surface	E_{ads} (eV)	$\vec{F}$	Cyclohexane	Surface	E_{ads} (eV)	$\vec{F}$	Cyclohexane	Surface	E_{ads} (eV)
0.6	↑	No	No	-0.38	↑	No	↑	-0.72	↑	No	↓	0.00
0.4	↑	No	No	-0.39	↑	No	↑	-0.60	↑	No	↓	-0.10
0.2	↑	No	No	-0.39	↑	No	↑	-0.48	↑	No	↓	-0.22
0	No	No	No	-0.39	No	No	↑	-0.36	No	No	↓	-0.37
-0.2	↓	No	No	-0.39	↓	No	↑	-0.24	↓	No	↓	-0.46
-0.4	↓	No	No	-0.40	↓	No	↑	-0.12	↓	No	↓	-0.58
-0.6	↓	No	No	-0.40	↓	No	↑	-0.01	↓	No	↓	-0.72

Table S4. Summary of electric field effects on the calculated adsorption energy, E_{ads}, for the nitric oxide molecule on pristine MoS_2 and Janus MoSSe monolayers.

E-field strength (V/Å)	MoS_2	MoSSe-S	MoSSe-Se
	NO	NO	NO
0.6	-0.16	-0.56	0.07
0.4	-0.15	-0.40	0.03
0.2	-0.15	-0.29	-0.08
0	-0.18	-0.19	-0.20
-0.2	-0.17	-0.07	-0.30
-0.4	-0.17	0.04	-0.41
-0.6	-0.18	0.11	-0.57

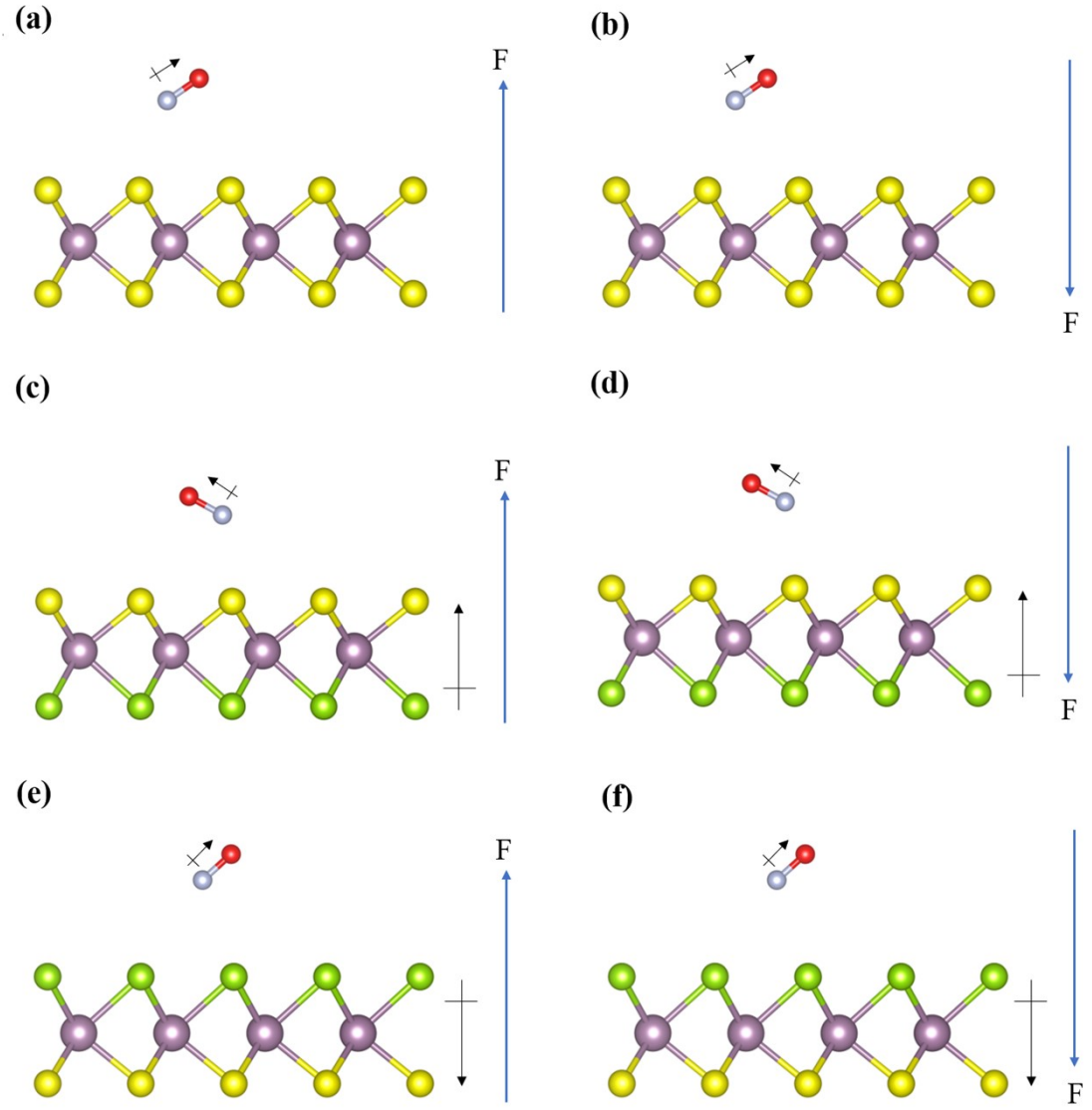

Figure S1. Optimized adsorption structures of nitric oxide molecule on the (a) MoS_2 with the positive external electric field, (b) MoS_2 with a negative external electric field, (c) S-layer of Janus MoSSe with the positive external electric field, (d) S-layer of Janus MoSSe with the negative external electric field, (e) Se-layer of Janus MoSSe with the positive external electric field, and (f) Se-layer of Janus MoSSe with the negative external electric field. The arrows are the directions of the dipole moment and the external electric field. Purple, yellow, and green spheres represent Mo, S, and Se atoms, respectively, while light blue and red balls are N and O atoms, respectively.

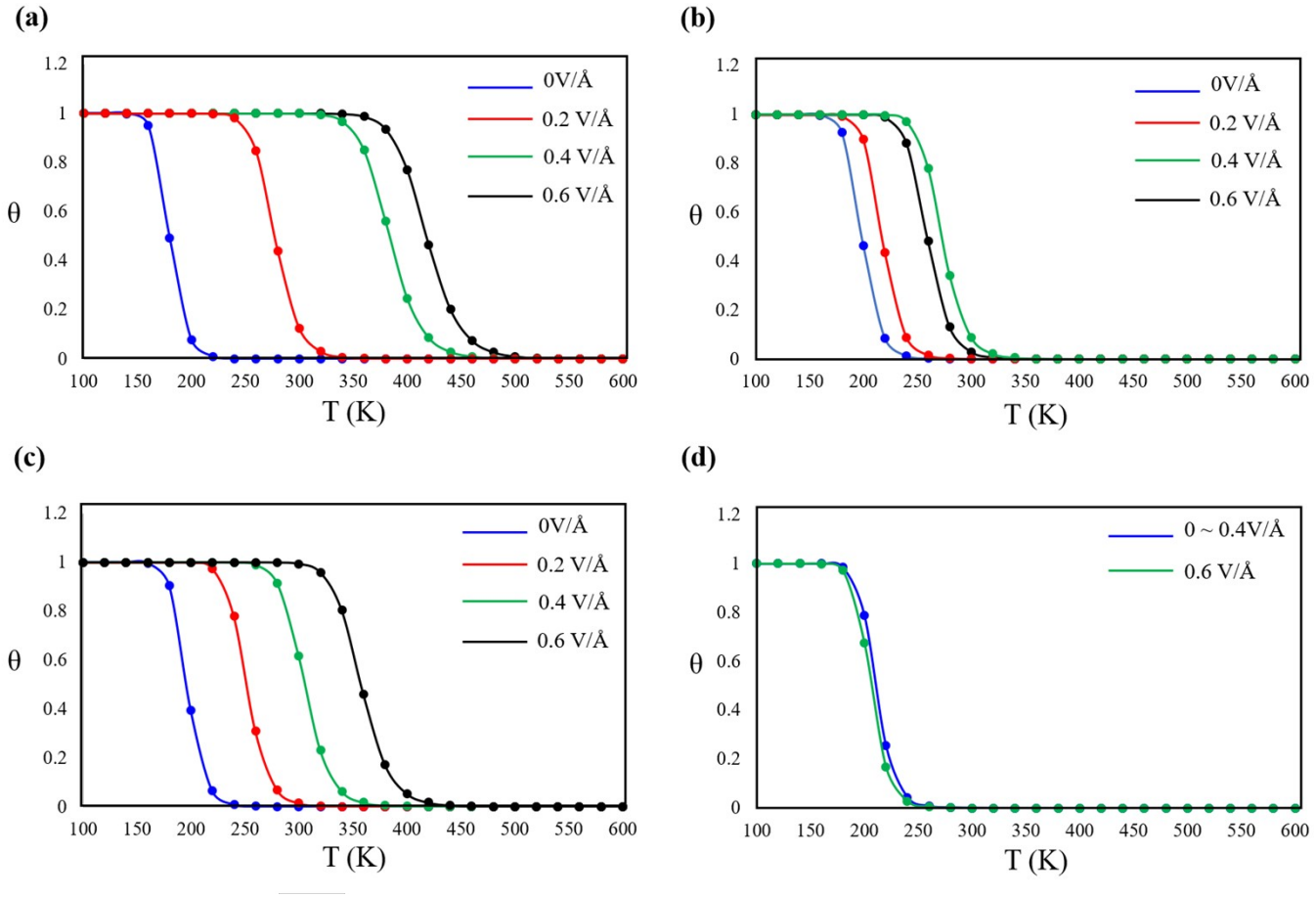

Figure S2. Calculated temperature evolution diagrams of different adsorbates coverage under different external electric fields: (a) acetone on Janus MoSSe, (b) acetone on MoS_2, (c) cyclohexane on Janus MoSSe, and (d) cyclohexane on MoS_2. $\theta = 1$ represents the fully occupied of the adsorbates while $\theta = 0$ means the empty surface, namely, all the adsorbates having been desorbed from the surface.

Microkinetic Simulations

All microkinetic simulations were performed using MKMCXX software. The rates of the adsorption (r_{ads}) and desorption (r_{des}) of species A can be defined as:

$$r_{ads}(t) = k_{ads} \times Y_A \times \theta \quad (1)$$

$$r_{des}(t) = k_{des} \times \theta_A \quad (2)$$

where k is the rate constant, θ is the coverage on the surface, and Y is mole fraction in the gas-phase. Adsorption and desorption can therefore be described by the same set of rate equations. The desorption rate is usually expressed by a rate law of nth order:

$$v = -\frac{d\theta}{dt} = k \times \theta^n \quad (3)$$

, and the rate law is usually referred to as the *Polanyi-Wigner* equation:

$$v = -\frac{d\theta}{dt} = k \times \theta^n = A(\theta,T) exp\left(\frac{-E_{des}(\theta,T)}{kT}\right) \times \theta^n \quad (4)$$

where $E_{des}(\theta,T)$ is the electronic energy for the desorption process and $A(\theta,T)$ is the pre-exponential factor.

For the desorption process of the adsorbates, we assume that the fully absorbed species only contain vibrational degrees of freedom. When the adsorbates desorb from the surface, the desorption rate constant can be written in the following expression:

$$k = \frac{k_b T}{h} \times \frac{Q_{trans}^{\ddagger(2)} Q_{rot}^{\ddagger(3)} Q_{vib}^{\ddagger(3N-6)}}{Q_{vib}^{(3N)}} \exp\left(\frac{-E_{des}}{k_b T}\right)$$

$$= \frac{k_b T}{h} \times \frac{A(2\pi m k_b T)}{h^2} \times \frac{8\pi^2 I k_b T}{\sigma h^2} \exp\left(\frac{-E_{des}}{k_b T}\right) \quad (5)$$

where the σ is the symmetry number and the $\frac{h^2}{8\pi^2 I k_b}$ is the rotational temperature θ_{rot}. Thus, the desorption rate constant is equal to:

$$k = \frac{k_b T^3}{h^3} \times \frac{A(2\pi m k_b)}{\sigma \theta_{rot}} exp\left(\frac{-E_{des}}{k_b T}\right) \quad (6)$$