Supporting Information for

Janus Monolayer of WSeTe, A New Structural Phase Transition Material Driven by Electrostatic Gating

Yajing Sun[†], Zhigang Shuai[†‡], and Dong Wang[*†]

[†]MOE Key Laboratory of Organic Opto Electronics and Molecular Engineering, Department of Chemistry, Tsinghua University, Beijing 100084, P R China

[‡]Key Laboratory of Organic Solids, Beijing National Laboratory for Molecular Science (BNLMS), Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, P R China

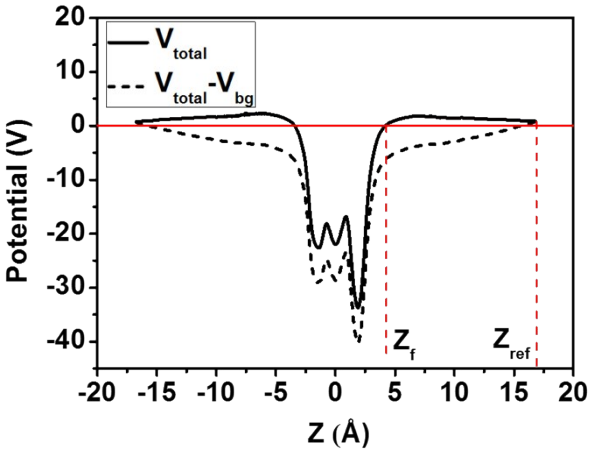

Figure S1 Plane-averaged electrostatic potential along the vacuum direction Z of a charged (0.05 e per formula unit) Janus monolayer of WSeTe in the H phase. The black solid line shows the total potential V_{total}, including the potential arising from the charged monolayer and that from the uniform compensating background charge V_{bg}. The dashed line shows the potential of the charged monolayer only, $V_{total} - V_{bg}$. The red line denotes the Fermi level μ_F of a charged system.

In a DFT calculation of a charged system with periodic boundary conditions, a homogeneous background charge is automatically introduced to compensate for the excess charge. We choose the middle plane of the vacuum slab as the reference plane. The reference plane is parallel to the monolayer, at a distance z_{ref} away from the Janus monolayer center. The energy of the charged monolayer $E_{mo}(Q, z_{ref})$ can be calculated by,[1]

$$E_{mo}(Q, z_{ref}) = E0 + \int_0^Q \Delta V(Q', z_{ref})\, dQ' \quad (1)$$

where $E0$ is the ground-state energy of an electrically neutral monolayer, the integral is the energy of moving charge Q' from the reference plane to the Fermi level of the monolayer, and $\Delta V(Q', z_{ref})$ is the electronic potential difference between the reference plane z_{ref} and the surface of the monolayer defined as z_f. As illustrated in Figure S1, z_f is the distance at which the total potential is equal to the Fermi level.

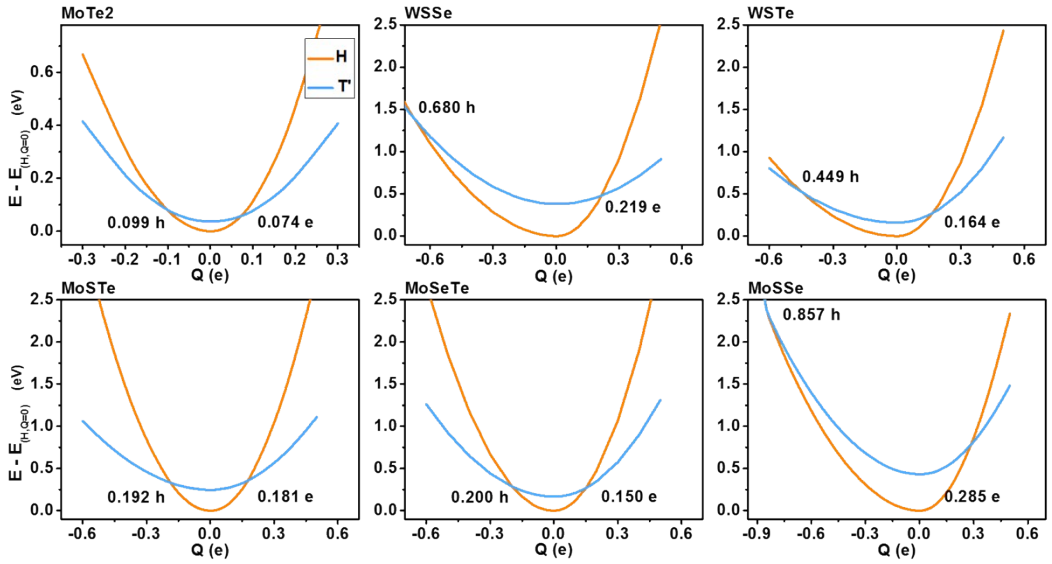

Figure S2 Energies of $MoTe_2$ and Janus monolayer MXY except for WSeTe in the H and T'phases respectively, as a function of the excessive charge.

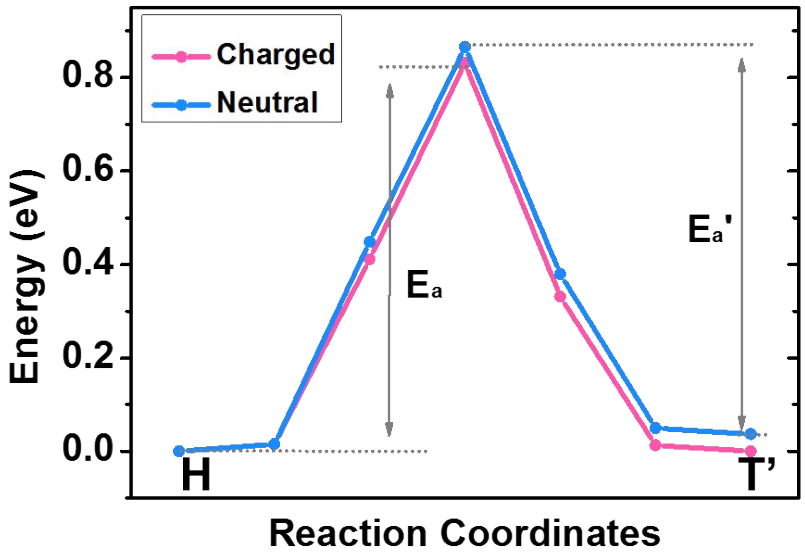

Figure S3 The NEB results of the phase transition barriers between T′ and H phases of $MoTe_2$ monolayer. E_a = 0.833 eV/f.u. is the kinetic barrier for the H-to-T' phase transition with $MoTe_2$ in the charged state (0.074 e/f.u. or 0.099 h/f.u. where H and T' phases are equally stable), and E_a' = 0.83 eV is the reversed T'-to-H transition barrier with $MoTe_2$ in the charge neutral state. These two barriers are related to the kinetics of the structural phase transition modulated by electrostatic doping in the FET device.

Table S1 Structural parameters and the total energy of $MoTe_2$ and six Janus monolayers of TMDCs in the H and T' phases, respectively. **a** and **b** are the lattice

parameters of the unit cell, **h** is the thickness of monolayers, referring to the height between the top-layer and bottom-layer chalcogen atoms, ΔE is the energy difference between H and T' phases, $E_{T'} - E_{H.}$

		a /Å	b /Å	Height (h) /Å	E /eV	ΔE / meV
MoTe2	H	3.522	\	3.620	-18.635	36
	T'	3.451	6.297	4.135	-18.598	
MoSSe	H	3.232	\	3.239	-21.181	432
	T'	3.199	5.837	3.609	-20.749	
MoSTe	H	3.339	\	3.385	-20.138	247
	T'	3.308	6.036	3.787	-19.891	
MoSeTe	H	3.406	\	3.620	-19.426	167
	T'	3.359	6.129	3.939	-19.259	
WSSe	H	3.231		3.252	-23.135	586
	T'	3.233	5.801	3.633	-22.548	
WSTe	H	3.340		3.396	-21.951	159
	T'	3.342	5.997	3.824	-21.792	
WSeTe	H	3.405		3.502	-21.182	48
	T'	3.390	6.083	3.982	-21.134	

Reference

(1) Li, Y.; Duerloo, K. A.; Wauson, K.; Reed, E. J. Structural Semiconductor-to-Semimetal Phase Transition in Two-Dimensional Materials Induced by Electrostatic Gating. *Nat Commun* **2016**, *7*, 10671.