Equibiaxial strain regulates the electronic structure, mechanical properties, piezoelectric, and thermal transport properties of 2Hphase monolayer CrX2 (X=S, Se, Te)

Shao-Bo Chen, ^{a†} San-Dong Guo, ^b Wan-Jun Yan, ^a Xiang-Rong Chen, ^{c‡} and Hua-Yun Geng, ^d

a College of Electronic and Information Engineering, Anshun University, Anshun 561000, People's Republic of China

b School of Electronic Engineering, Xi'an University of Posts and Telecommunications, Xi'an 710121, People's Republic of China

c College of Physics, Institute of Atomic and Molecular Physics, Sichuan University,

Chengdu 610065, People's Republic of China

d National Key Laboratory for Shock Wave and Detonation Physics Research, Institute

of Fluid Physics, CAEP, Mianyang 621900, People's Republic of China



Fig. S1 Top and side view of the different structures for the CrS_2 monolayer. (a) Top and (b) side view of 2H phase CrS_2 monolayer; (c) Top and (d) side view of 1T phase CrS_2 monolayer; (e) Top and (f) side view of 1T' phase CrS_2 monolayer.

Table S1 The calculation of the total energy and cohesive energy for 2H, 1T, and 1T' structures.

Compounds	2Н		1T		1T '	
	Total	Cohesive	Total	Cohesive	Total	Cohesive
	energy	energy	energy	energy	energy	energy
	(eV)	(eV/atom)	(eV)	(eV/atom)	(eV)	(eV/atom)
CrS ₂	-19.77	-1.47	-19.25	-1.53	-19.44	-1.31
CrSe ₂	-17.97	-0.94	-17.54	-1.36	-17.80	-1.14
CrTe ₂	-16.05	-0.53	-15.76	-0.90	-16.09	-0.79



Fig. S2 The various strain energy (black square) with biaxial strain, and the quadratic

fitting (red line) of strain energy.

Compounds	Strain	PBE	PBE+SOC	HSE+SOC
CrS ₂	-0.02	1.15d	1.11d	2.06d
	0	1.01d	0.98d	1.99d
		1.07d[1]	0.951d[2]	1.75d[3] (HSE
		(LDA+U)	(PBE+SOC)	$+G_0W_0)$
	0.02	0.90d	0.87d	1.86d
	0.04	0.63i	0.63i	1.72i
	0.06	0.39i	0.39i	1.63i
	0.08	0.19i	0.19i	1.58i
	-0.02	0.85d	0.80d	2.01d
		0.86d		
		[1] (LDA+U		
CrSe ₂)		
	0	0.75d	0.70d	1.94d
	0.02	0.67d	0.63d	1.79i
	0.04	0.47i	0.46i	1.68i
	0.06	0.28i	0.38i	1.20i
	0.08	0.12i	0.12i	0.45i
CrTe ₂	-0.02	0.60d	0.54d	1.74d

Table S2 The calculated bandgap at PBE, PBE+SOC, and HSE+SOC levels.

0	0.53d	0.47d	1.62d
	0.60 [1]		
	(LDA+U)		
0.02	0.47d	0.41d	0.82d
0.04	0.39i	0.37i	0.71d
0.06	0.23i	0.19i	0.62i

All our values of bandgap are calculated by projector-augmented wave (PAW) potentials with PBE exchange-correlation potential. We also made a comparison with other results calculated by different potentials, methods, and parameter settings. In Table 1, d and i represent the direct bandgap and indirect bandgap, respectively. Notably, the spin-orbit coupling effect of Cr does have less effect on the bandgap.

To obtain detailed bandgap information, the band structures with PBE and PBE+SOC levels are calculated, as listed in Table S2 in the supplemental materials. By comparison, our computer results agree with other references, and the spin-orbit coupling effect of Cr does have less effect on the bandgap. The band gap of CrS_2 is 1.99 eV higher than 1.75 eV in reference [3]. To further explain this difference, we compare the differences in the calculation process of the two in detail. It is found that the band structure is computed by the [3] HSE06+GW method, while we use the HSE06+SOC method to calculate the band structures for CrX_2 monolayers. In addition, the values of the cutoff energy and k-point are different. Last but not least, the lattice constant are little different and very sensitive to affect the size of the bandgap.

References:

[1] C. Ataca, H. Şahin, S. Ciraci, Stable, single-layer MX_2 transition-metal oxides and dichalcogenides in a honeycomb-like structure, J. Phys. Chem. C, 116 (2012) 8983-8999.

[2] M.R. Habib, S. Wang, W. Wang, H. Xiao, S.M. Obaidulla, A. Gayen, Y. Khan, H. Chen, M. Xu, Electronic properties of polymorphic two-dimensional layered chromium disulphide, Nanoscale, 11 (2019) 20123-20132.

[3] H.L. Zhuang, M.D. Johannes, M.N. Blonsky, Computational prediction and characterization of single-layer CrS_2 , Appl. Phys. Lett., 104 (2014) 022116.