补充材料

结构相变引起单层 $RuSe_2$ 载流子迁移率的提高*

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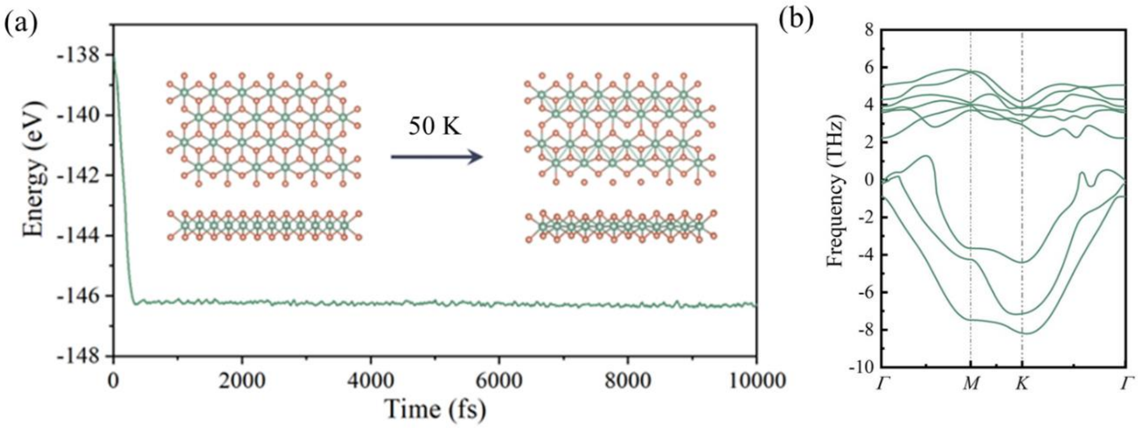

图 S1 (a) AIMD 模拟 50 K 时 *T* 相单层 $RuSe_2$ 总能量随时间的变化；（b）*T* 相单层 $RuSe_2$ 的声子谱

FigS1. (a) Variation of the total energy of monolayer T-phase $RuSe_2$ with time during AIMD simulation at 50 K; (b) phonon spectrum of monolayer T-phase $RuSe_2$.

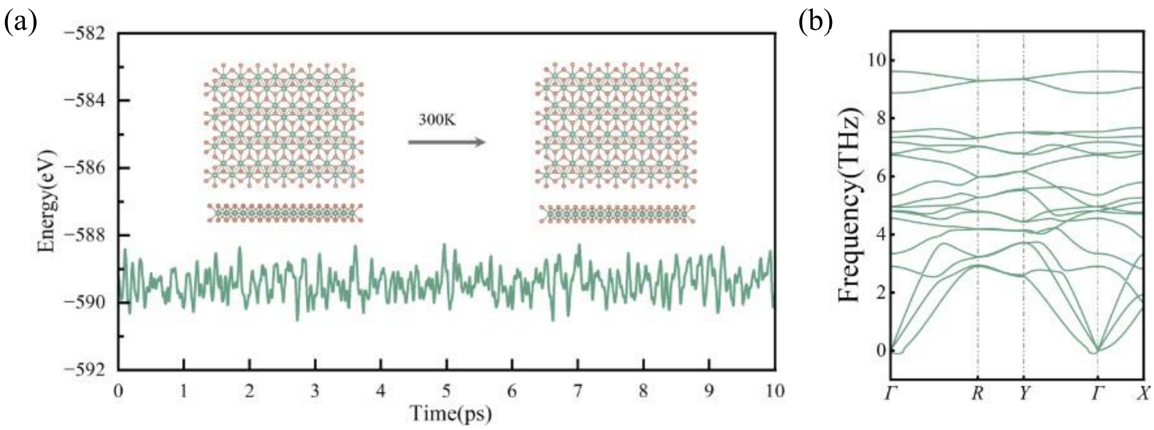

图 S2 (a)AIMD 模拟 300 K 时 *T′*相单层 $RuSe_2$ 总能量随时间的变化；(b)*T′*相单层 $RuSe_2$ 的声子谱

FigS2. (a) Variation of the total energy of monolayer *T′*-phase $RuSe_2$ with time during AIMD simulation at 300 K; (b) phonon spectrum of monolayer *T′*-phase $RuSe_2$.

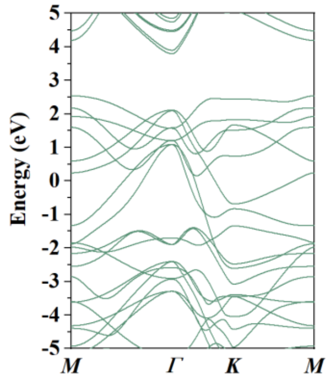

图 S3 *H* 相 $RuSe_2$ 单层能带图

Fig.S3. Band structure diagram of monolayer *H*-phase $RuSe_2$.

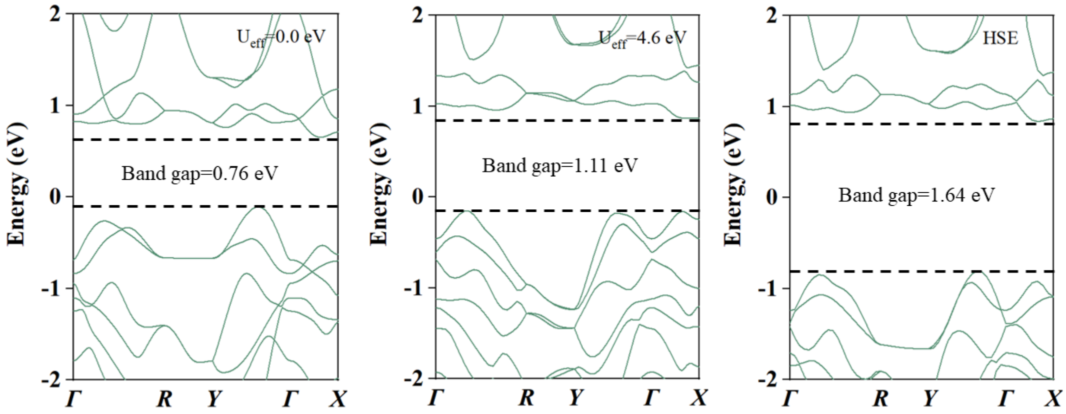

图 S4 T′相 RuSe2 的能带结构图，从左往右分别为 U_{eff}=0 eV，U_{eff}=4.6 eV 以及 HSE 的计算结果

Fig.S4. Band structure diagram of *T′*-phase $RuSe_2$, from left to right, represents the calculation results of U_{eff}=0 eV, U_{eff}=4.6 eV, and HSE.

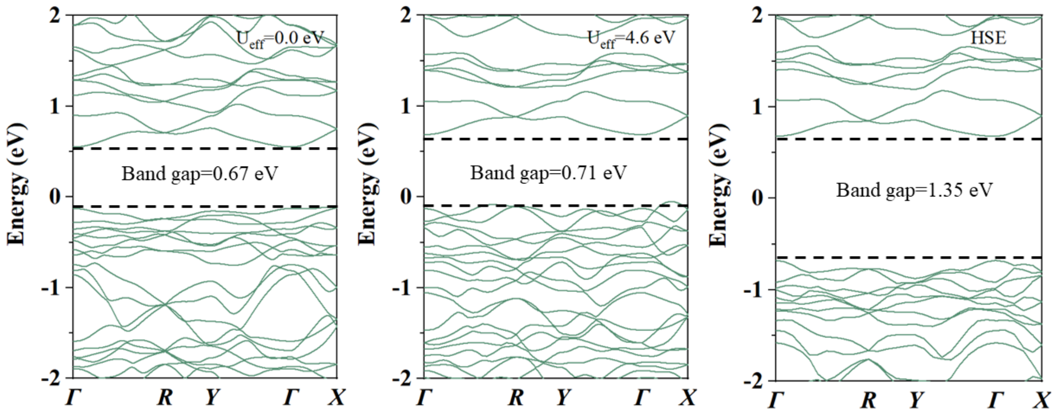

图 S5 T′′′相 RuSe2 的能带结构图，从左往右分别为 U_{eff}=0 eV，U_{eff}=4.6 eV 以及 HSE 的计算结果

Fig.S5. Band structure diagram of *T′′′*-phase $RuSe_2$, from left to right, represents the calculation results of U_{eff}=0 eV, U_{eff}=4.6 eV, and HSE.

表 S1 从我们的计算中获得的单层 $RuSe_2$ 两种畸变相的原子位置，位置坐标以分数坐标的形式表示，z 轴的晶格长度取为 20 Å

Table S1. Atomic positions of the two distortion phases of monolayer RuSe2 obtained from our calculations, the values given here are represented in the form of fractional coordinates, the lattice parameter along the z-axis is taken as 20 Å.

Phase	Site	Wyckoff symbol	*x*	*y*	*z*
T′	Ru_1	2e	0.304	0.750	0.501
	Ru_2	2e	0.695	0.250	0.498
	Se_1	2e	0.591	0.750	0.416
	Se_2	2e	0.408	0.250	0.583
	Se_3	2e	0.089	0.250	0.436
	Se_4	2e	0.910	0.750	0.563
T‴	Ru_1	4f	0.492	0.386	0.234
	Ru_2	4f	0.507	0.613	0.765
	Ru_3	4f	0.507	0.886	0.765
	Ru_4	4f	0.492	0.113	0.234
	Ru_5	2e	0.494	0.250	0.826
	Ru_6	2e	0.505	0.750	0.173
	Se_1	4f	0.434	0.425	0.608
	Se_2	4f	0.565	0.574	0.391
	Se_3	4f	0.565	0.925	0.391
	Se_4	4f	0.434	0.074	0.608
	Se_5	4f	0.428	0.921	0.069
	Se_6	4f	0.571	0.078	0.930
	Se_7	4f	0.571	0.421	0.930
	Se_8	4f	0.428	0.578	0.069
	Se_9	2e	0.403	0.250	0.098
	Se_{10}	2e	0.596	0.750	0.901
	Se_{11}	2e	0.565	0.250	0.461
	Se_{12}	2e	0.434	0.750	0.538

