

补充材料

结构相变引起单层 RuSe₂ 载流子迁移率的提高*

陆康俊, 王一帆, 夏谦[†], 张贵涛, 陈乾[†]

(东南大学物理学院, 量子材料与信息器件教育部重点实验室, 南京 211189)

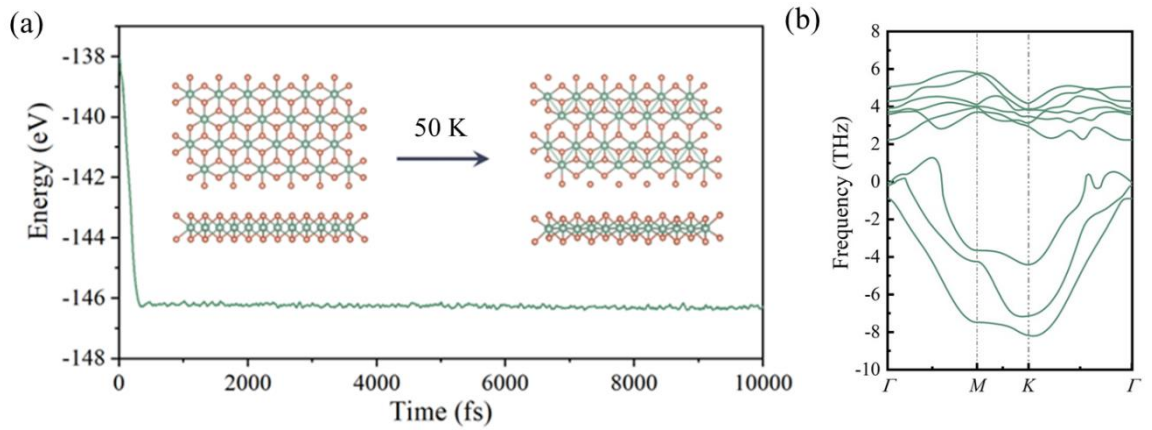


图 S1 (a) AIMD 模拟 50 K 时 *T* 相单层 RuSe₂ 总能量随时间的变化; (b) *T* 相单层 RuSe₂ 的声子谱

FigS1. (a) Variation of the total energy of monolayer *T*-phase RuSe₂ with time during AIMD simulation at 50 K; (b) phonon spectrum of monolayer *T*-phase RuSe₂.

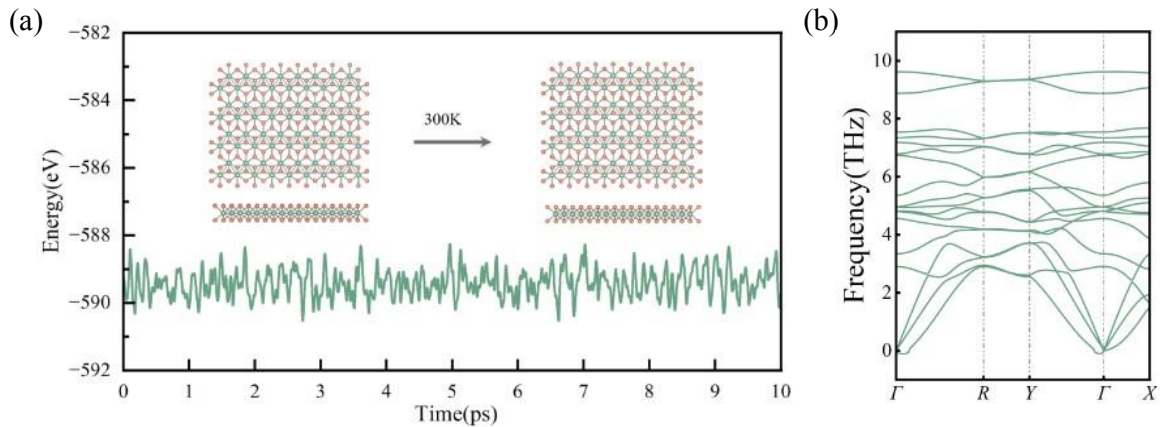


图 S2 (a) AIMD 模拟 300 K 时 *T'* 相单层 RuSe₂ 总能量随时间的变化; (b) *T'* 相单层 RuSe₂ 的声子谱

FigS2. (a) Variation of the total energy of monolayer *T'*-phase RuSe₂ with time during AIMD simulation at 300 K; (b) phonon spectrum of monolayer *T'*-phase RuSe₂.

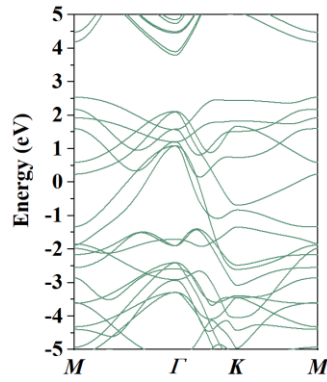


图 S3 H 相 RuSe_2 单层能带图

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

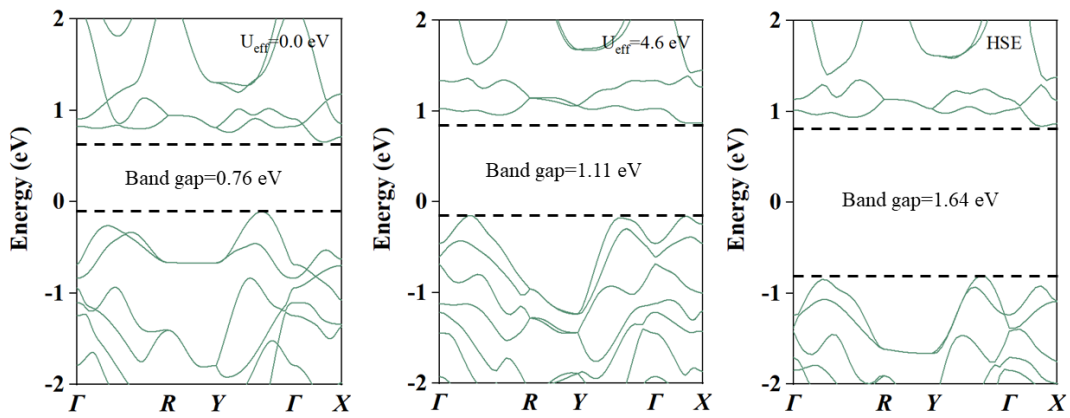


图 S4 T' 相 RuSe_2 的能带结构图，从左往右分别为 $U_{\text{eff}}=0 \text{ eV}$ ， $U_{\text{eff}}=4.6 \text{ eV}$ 以及 HSE 的计算结果

Fig.S4. Band structure diagram of T' -phase RuSe_2 , from left to right, represents the calculation results of $U_{\text{eff}}=0 \text{ eV}$,

$U_{\text{eff}}=4.6 \text{ eV}$, and HSE.

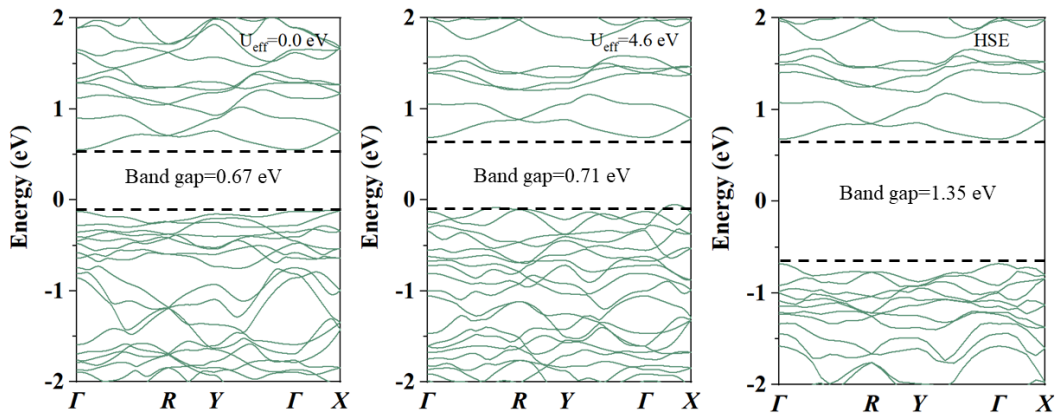


图 S5 T''' 相 RuSe_2 的能带结构图，从左往右分别为 $U_{\text{eff}}=0 \text{ eV}$ ， $U_{\text{eff}}=4.6 \text{ eV}$ 以及 HSE 的计算结果

Fig.S5. Band structure diagram of T''' -phase RuSe_2 , from left to right, represents the calculation results of $U_{\text{eff}}=0$

eV , $U_{\text{eff}}=4.6 \text{ eV}$, and HSE.

表 S1 从我们的计算中获得的单层 RuSe₂ 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	