

《二维范德华异质结 $\text{Cs}_3\text{X}_2\text{I}_9/\text{InSe}$ ($X = \text{Bi}, \text{Sb}$) 的光电性能*》 的补充材料

熊祥杰¹⁾ 钟防¹⁾ 张资文¹⁾ 陈芳¹⁾ 罗婧澜²⁾

赵宇清^{1)†} 朱慧平^{3)‡} 蒋绍龙^{4)††}

- 1) (湖南科技大学物理与电子科学学院, 智能传感器与新型传感器材料湖南省重点实验室, 湘潭 411201)
- 2) (格拉斯哥大学亚当史密斯学院, 格拉斯哥 G12 8QQ)
- 3) (中国科学院微电子研究所, 硅器件技术重点实验室, 北京 100029)
- 4) (粤港澳大湾区(广东)量子科学中心, 深圳 518045)

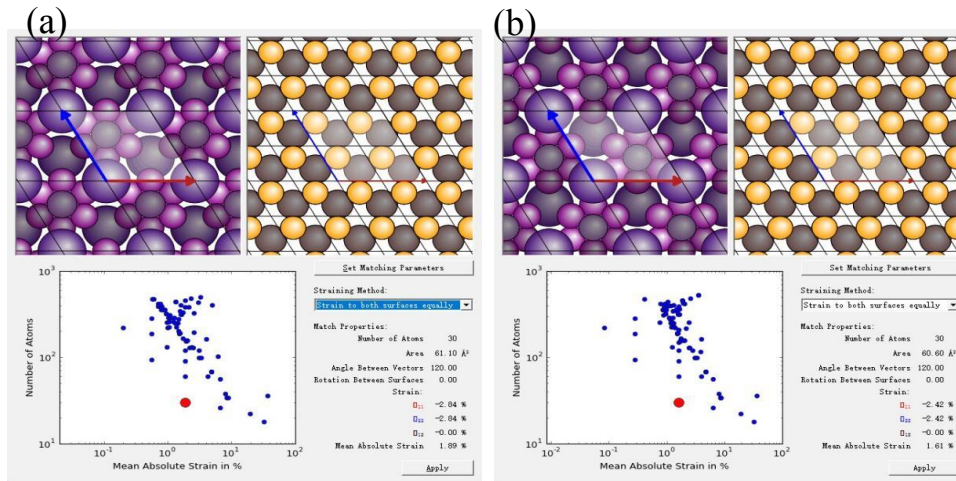


图 S1 (a) $\text{Cs}_3\text{Bi}_2\text{I}_9/\text{InSe}$ 和(b) $\text{Cs}_3\text{Sb}_2\text{I}_9/\text{InSe}$ 的晶格失配比图

Fig. S1. Lattice mismatch ratios of (a) $\text{Cs}_3\text{Bi}_2\text{I}_9/\text{InSe}$ and (b) $\text{Cs}_3\text{Sb}_2\text{I}_9/\text{InSe}$.

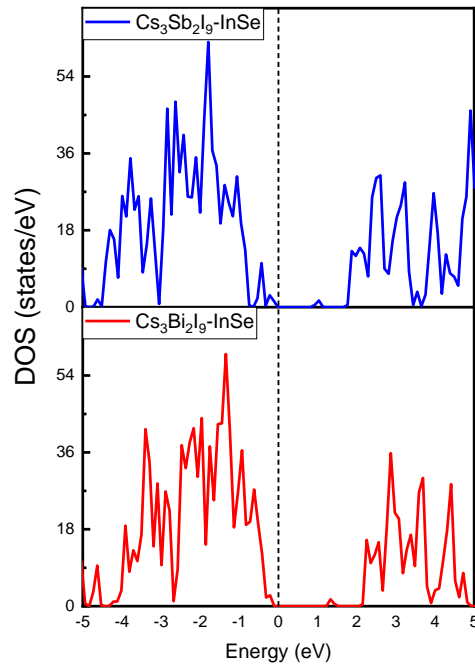


图 S2 二维 $\text{Cs}_3\text{X}_2\text{I}_9\text{-InSe}$ 异质结的态密度图

Fig. S2. Density of states of 2D $\text{Cs}_3\text{X}_2\text{I}_9\text{-InSe}$ heterostructure.

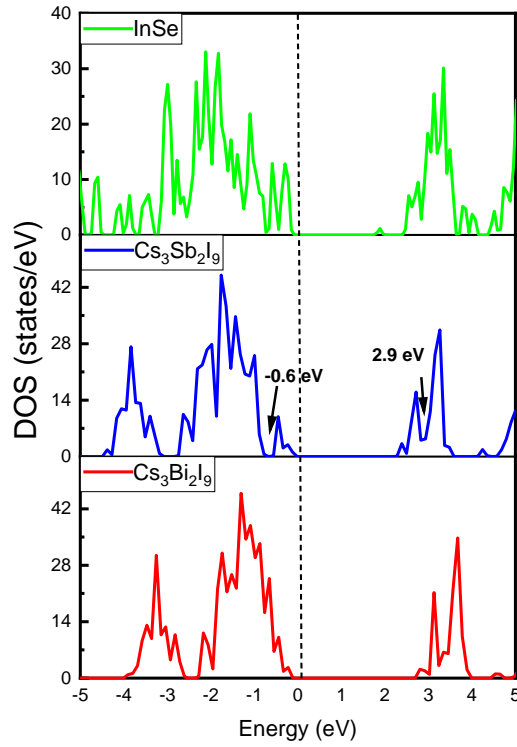


图 S3 单体结构 $\text{Cs}_3\text{Bi}_2\text{I}_9$, $\text{Cs}_3\text{Sb}_2\text{I}_9$ 和 InSe 的态密度图

Fig. S3. Density of states of free-standing monolayer $\text{Cs}_3\text{Bi}_2\text{I}_9$, $\text{Cs}_3\text{Sb}_2\text{I}_9$ and InSe .

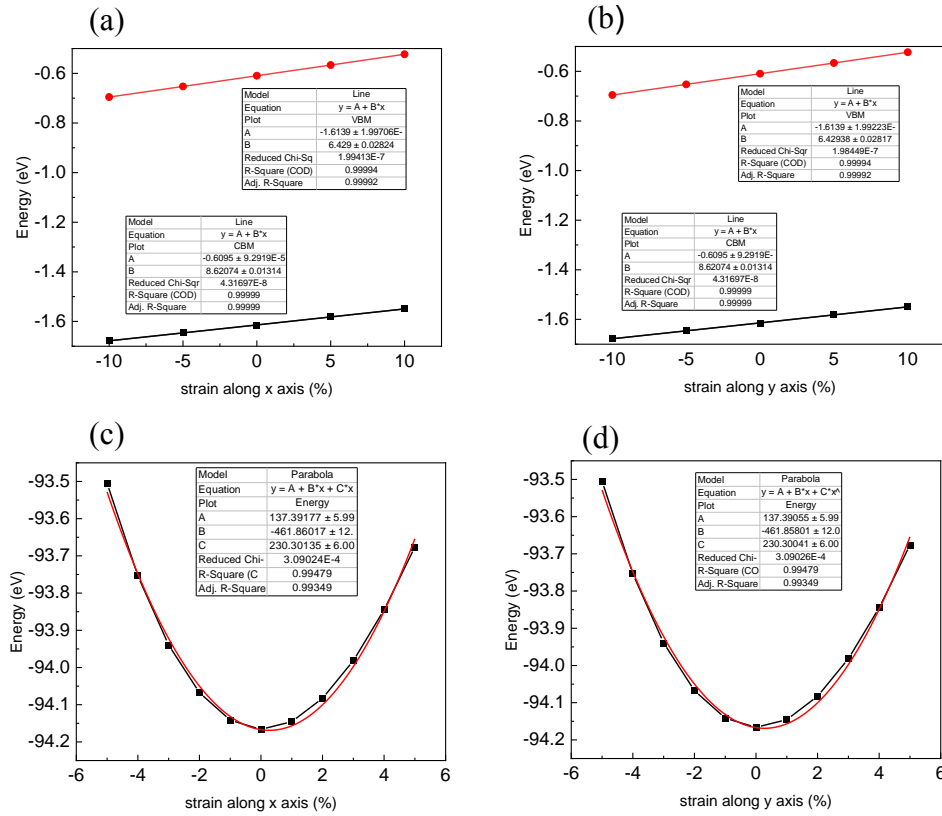


图 S4 沿(a) x 轴和(b) y 轴方向的二维 $\text{Cs}_3\text{Bi}_2\text{I}_9/\text{InSe}$ 的导带底(CBM)和价带顶(VBM)随晶格形变的线性拟合; 二维 $\text{Cs}_3\text{Bi}_2\text{I}_9/\text{InSe}$ 总能量与沿(c) x 轴和(d) y 轴方向晶格形变的二阶抛物线拟合

Fig. S4. Linear fits of the conduction band minimum (CBM) and valence band maximum (VBM) of 2D $\text{Cs}_3\text{Bi}_2\text{I}_9/\text{InSe}$ along (a) x -axis and (b) y -axis directions with lattice deformation. Parabolic fits of the total energy of 2D $\text{Cs}_3\text{Bi}_2\text{I}_9/\text{InSe}$ along (c) x -axis and (d) y -axis directions with lattice deformation.

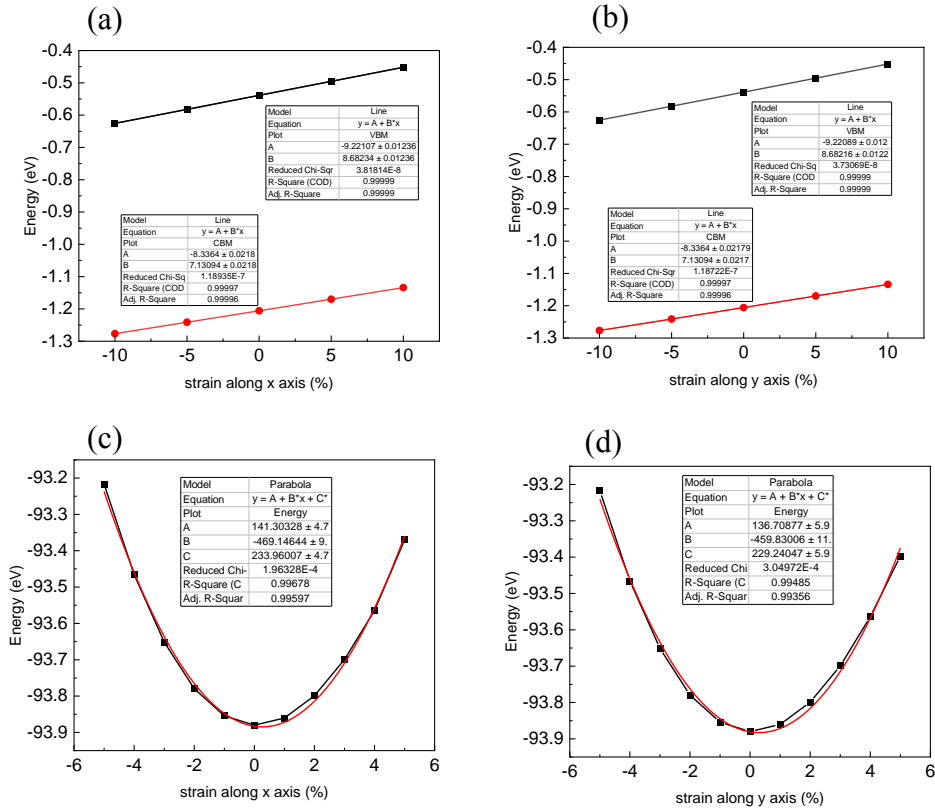


图 S5 沿(a) x 轴和(b) y 轴方向的二维 $\text{Cs}_3\text{Sb}_2\text{I}_9/\text{InSe}$ 的导带底(CBM)和价带顶(VBM)随晶格形变的线性拟合. 二维 $\text{Cs}_3\text{Sb}_2\text{I}_9/\text{InSe}$ 总能量与沿(c) x 轴和(d) y 轴方向晶格形变的二阶抛物线拟合

Fig. S5. Linear fits of the conduction band minimum (CBM) and valence band maximum (VBM) of 2D $\text{Cs}_3\text{Sb}_2\text{I}_9/\text{InSe}$ along (a) x -axis and (b) y -axis directions with lattice deformation. Parabolic fits of the total energy of 2D $\text{Cs}_3\text{Sb}_2\text{I}_9/\text{InSe}$ along (c) x -axis and (d) y -axis directions with lattice deformation.

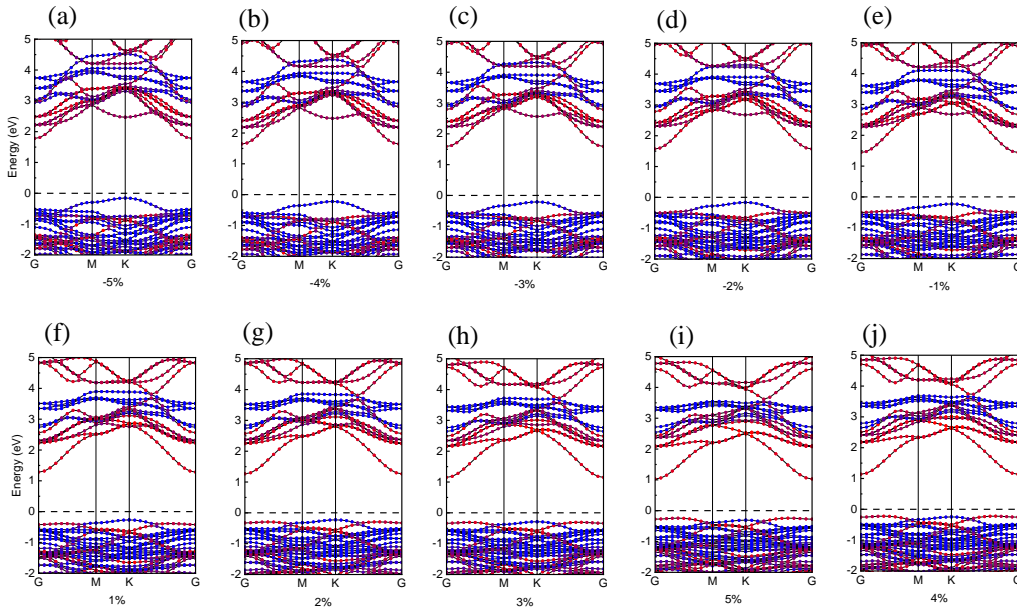


图 S6 (a) -5%, (b) -4%, (c) -3%, (d) -2%, (e) -1%, (f) +1%, (g) +2%, (h) +3%, (i) +4%, (j) +5% 双轴应变下的二维 $\text{Cs}_3\text{Bi}_2\text{I}_9/\text{InSe}$ 异质结的能带结构

Fig. S6. Band structures of 2D $\text{Cs}_3\text{Bi}_2\text{I}_9/\text{InSe}$ heterostructure under (a) -5%, (b) -4%, (c) -3%, (d) -2%, (e) -1%, (f) +1%, (g) +2%, (h) +3%, (i) +4%, (j) +5% biaxial strain.

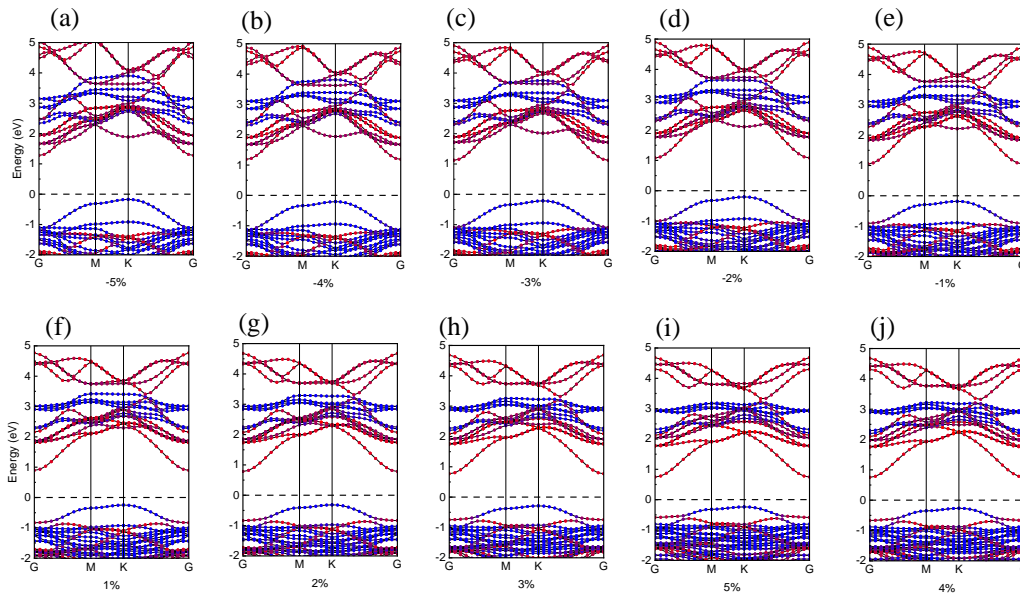


图 S7 (a) -5%, (b) -4%, (c) -3%, (d) -2%, (e) -1%, (f) +1%, (g) +2%, (h) +3%, (i) +4%, (j) +5% 双轴应变下的的二维 $\text{Cs}_3\text{Sb}_2\text{I}_9/\text{InSe}$ 异质结的能带结构

Fig. S7. Band structures of 2D $\text{Cs}_3\text{Sb}_2\text{I}_9/\text{InSe}$ heterostructure under (a) -5%, (b) -4%, (c) -3%, (d) -2%, (e) -1%, (f) +1%, (g) +2%, (h) +3%, (i) +4%, (j) +5% biaxial strain.