

《单层 CrI₃ 电荷输运性质和光学性质应变调控的第一性原理》的补充材料

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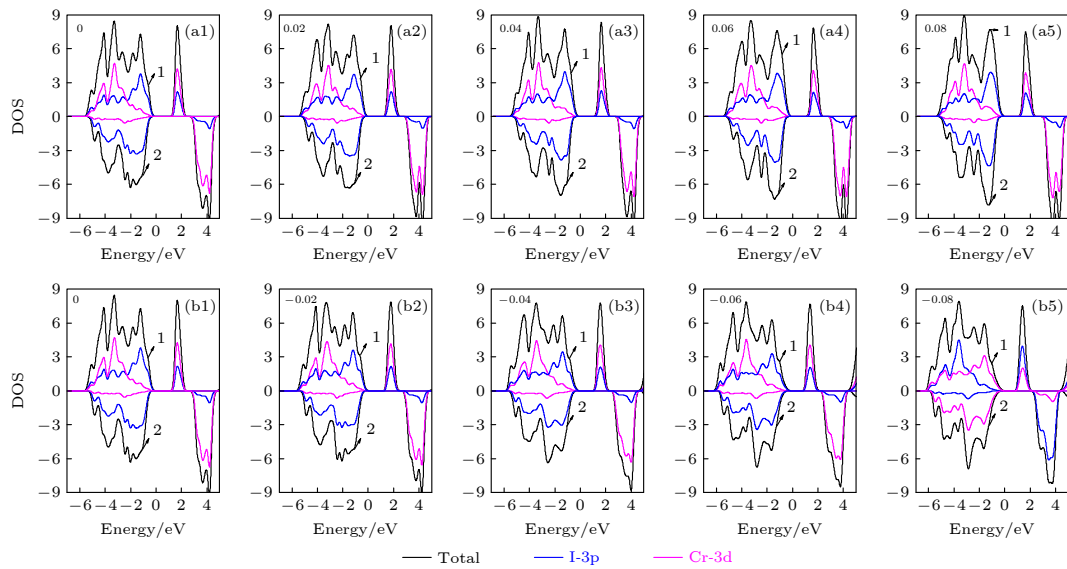


图 S1 锯齿型应变下 CrI₃ 的 DOS 图

Fig. S1. Zigzag strain dependence of DOS of CrI₃ monolayer.

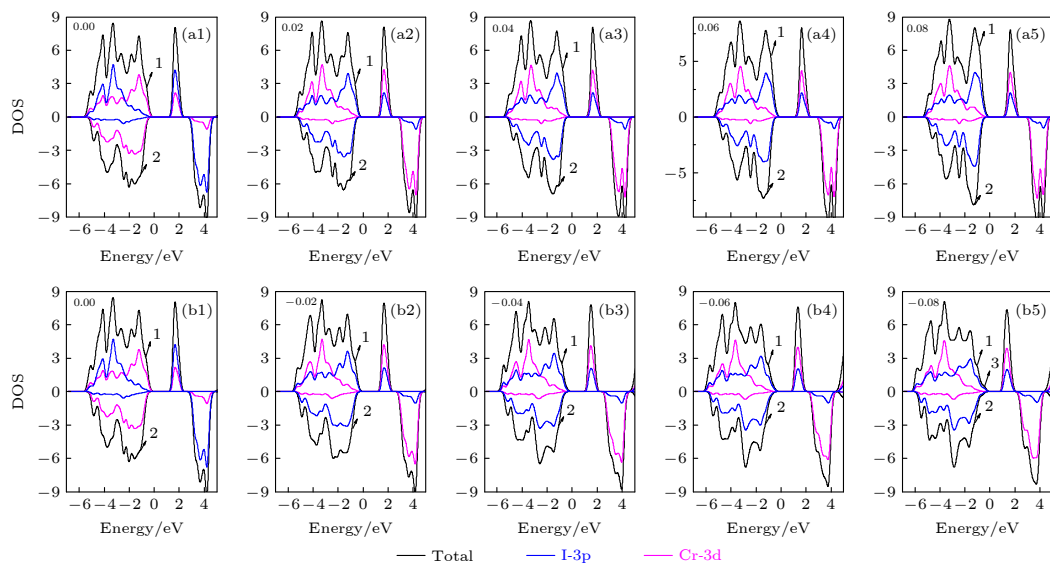


图 S2 扶手椅型应变下 CrI₃ 的 DOS 图

Fig. S2. Armchair strain dependence of DOS of CrI₃ monolayer.

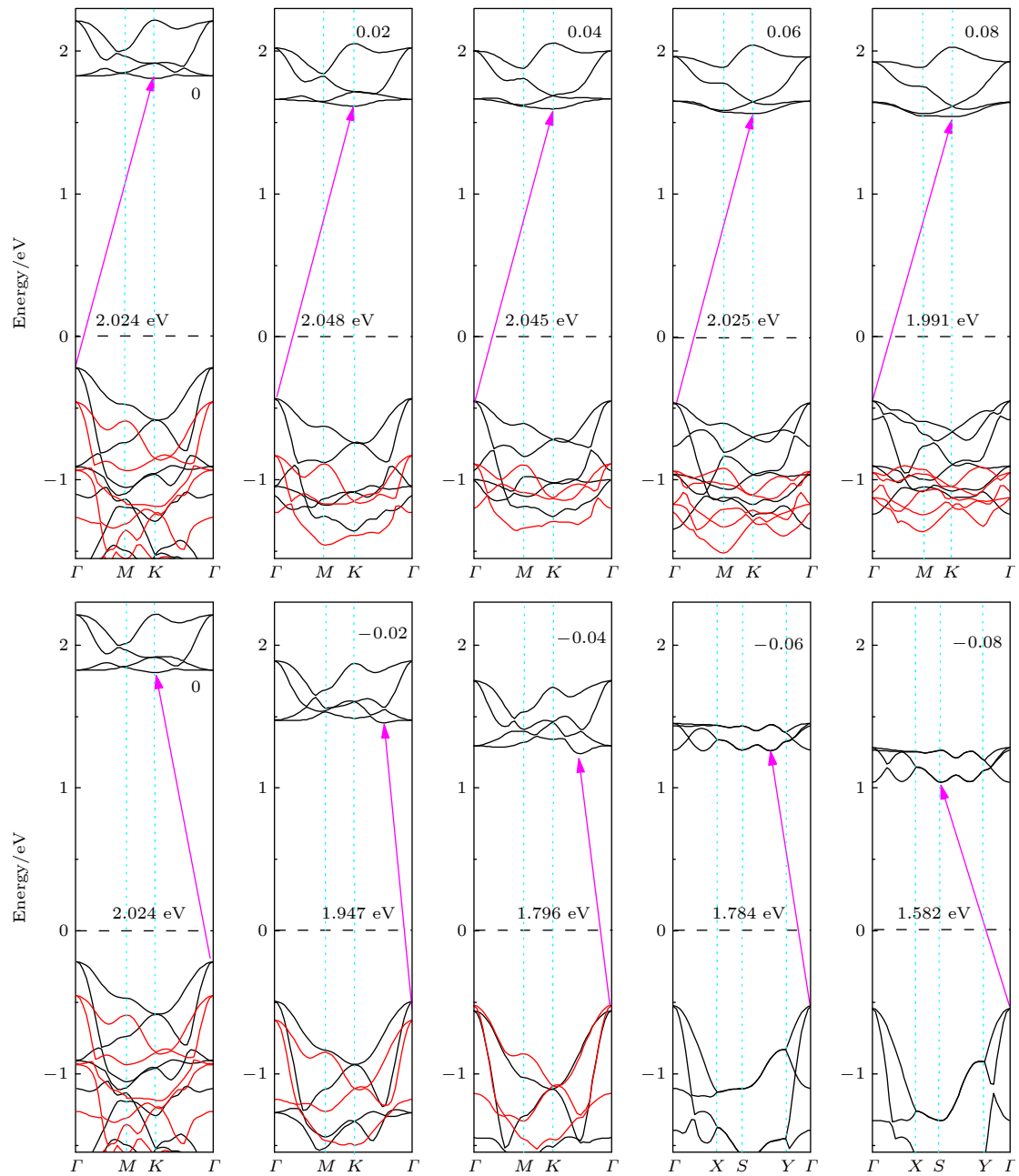


图 S3 双轴应变下 CrI_3 的能带结构图，黑色(红色)曲线代表极化向上(向下)能带

Fig. S3. Biaxial strain dependence of band structures of CrI_3 monolayer, with black (red) lines represent the spin-up (spin-down) band structure.

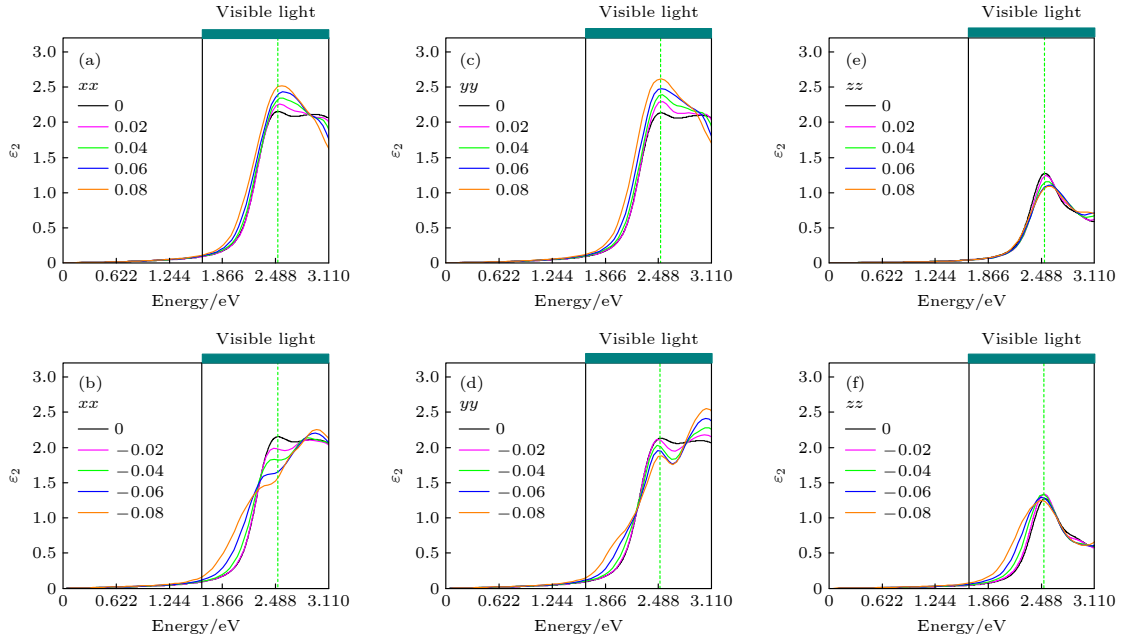


图 S4 锯齿型单轴应变下的介电函数虚部 (a), (c), (e) 拉伸应变; (b), (d), (f) 压缩应变

Fig. S4. Zigzag strain dependence of imaginary component of dielectric function: (a), (c), (e)

Tensile strain; (b), (d), (f) compressive strain.

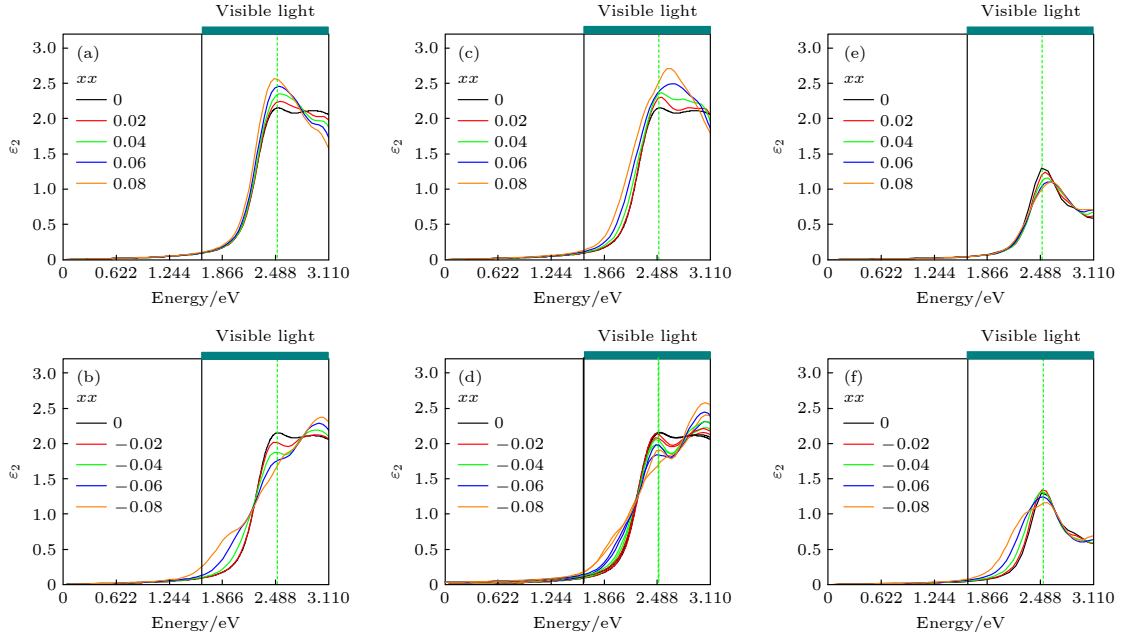


图 S5 扶手椅型单轴应变下的介电常数虚部 (a), (c), (e) 拉伸应变; (b), (d), (f) 压缩应变

Fig. S5. Armchair strain dependence of imaginary component of dielectric function: (a), (c), (e)

Tensile strain; (b), (d), (f) compressive strain.