补充材料

基于 MXene 涂层保护 Cs_3Sb 异质结光阴极材料的计算筛选*

白亮 [1)] 赵启旭 [1)] 沈健伟 [1)] 杨岩 [1)] 袁清红 [1)]

钟成 [2)] 孙海涛 [1)3)†] 孙真荣 [1)3)†]

1)（华东师范大学，精密光谱科学与技术国家重点实验室，上海 200241）

2)（武汉大学，化学与分子科学学院，武汉 430072）

3)（山西大学，极端光学协同创新中心，太原 030006）

图 S1—S7 分别为 M_2CF_2/M_2CF_2-Cs_3Sb，M_2CO_2/M_2CO_2-Cs_3Sb，$M_2C(OH)_2$/$M_2C(OH)_2$-Cs_3Sb，M_2CCl_2/M_2CCl_2-Cs_3Sb，M_2CS_2/M_2CS_2-Cs_3Sb，$M_2C(OCH_3)_2$/$M_2C(OCH_3)_2$-Cs_3Sb，$M_2C(NH)_2$/$M_2C(NH)_2$-Cs_3Sb 结构的功函数随原子序数变化示意图。图 S8 为 $Nb_{n+1}C_nT_2$ (n = 1，3，4)结构和 $Nb_{n+1}C_nT_2$-Cs_3Sb 异质结结构的功函数随 Nb/C 原子比例变化示意图。图 S9 为 $Ta_{n+1}C_nT_2$(n = 1，2，3)结构和 $Ta_{n+1}C_nT_2$-Cs_3Sb 异质结结构的功函数随 Ta/C 原子比例变化示意图。图 S10 为 $Ti_{n+1}C_nT_2$(n = 1，2，3，4)结构和 $Ti_{n+1}C_nT_2$-Cs_3Sb 异质结结构的功函数随 Ti/C 原子比例变化图。图 S11 为 M_2CT_2 结构的功函数随金属 M 原子变化示意图。图 S12 为 M_2CT_2-Cs_3Sb 结构的功函数随 M_2CT_2 结构功函数的变化示意图。图 S13 为 M_2CT_2-Cs_3Sb 结构的功函数随 M_2CT_2 结构的电离能(IP)变化示意图。图 14 为 V_2C-Cs_3Sb 异质结的差分电荷密度图和能级校正分析示意图, 等值面设为 0.001 e/bohr^3。图 15 为 V_2CO_2-Cs_3Sb 异质结的差分电荷密度图和能级校正分析示意图（等值面设为 0.003 e/bohr^3）。图 16 为 V_2CCl_2-Cs_3Sb 异质结的差分电荷密度图和能级校正分析示意图（等值面设为 0.001 e/bohr^3）。图 17 为 V_2CS_2-Cs_3Sb 异质结的差分电荷密度图和能级校正分析示意图（等值面设为 0.0015 e/bohr^3）。图 18 为 $V_2C(OCH_3)_2$-Cs_3Sb 异质结的差分电荷密度图和能级校正分析示意图（等值面设为 0.002 e/bohr^3）。图 S19 为 $V_2C(NH)_2$-Cs_3Sb 异质结的差分电荷密度图和能级校正分析示意图（等值面设为 0.0015 e/bohr^3）。

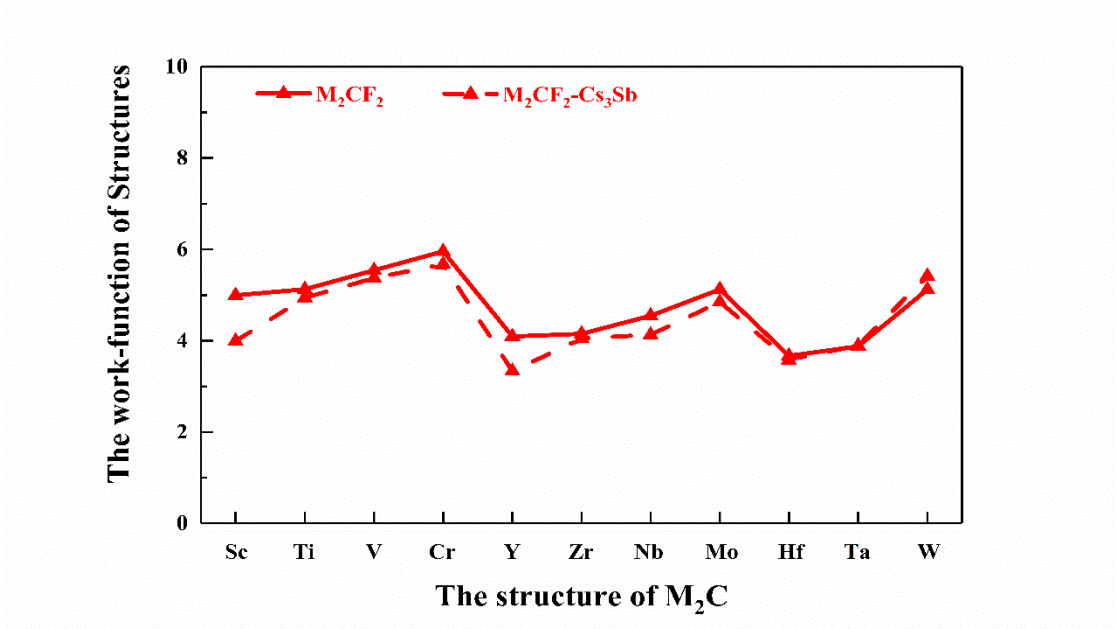


图 S1 M_2CF_2/M_2CF_2-Cs_3Sb结构的功函数随原子序数变化图

Fig. S1. Work-function of M_2CF_2 and M_2CF_2-Cs_3Sb structure vary with element number.

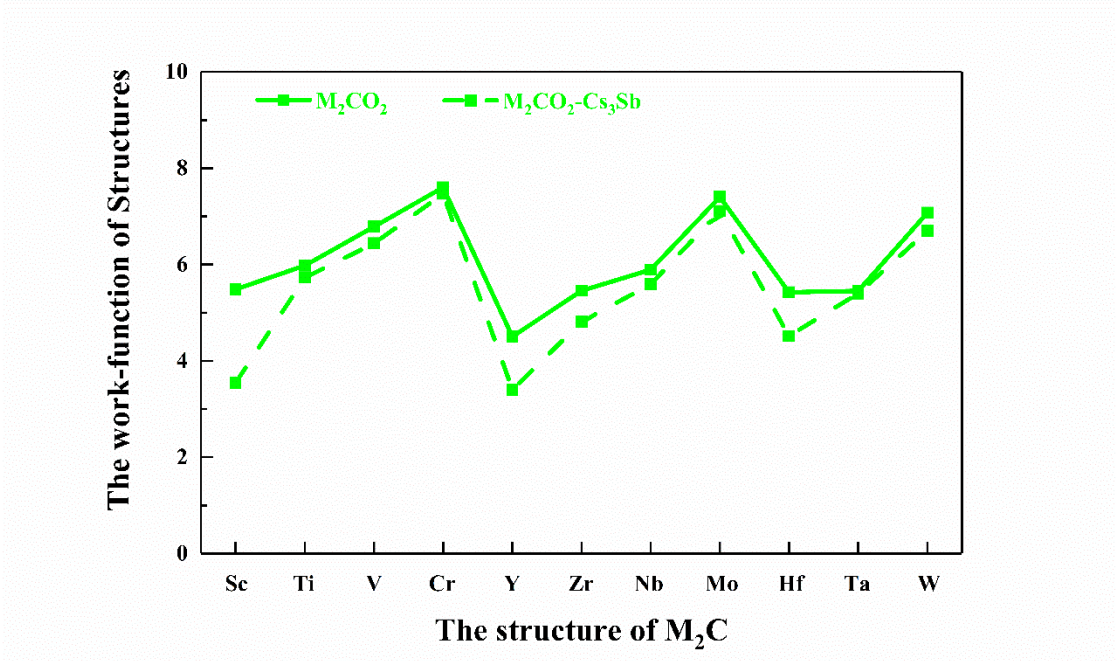


图 S2 M_2CO_2/M_2CO_2-Cs_3Sb结构的功函数随原子序数变化图

Fig. S2. Work-function of M_2CO_2 and M_2CO_2-Cs_3Sb structure vary with element number.

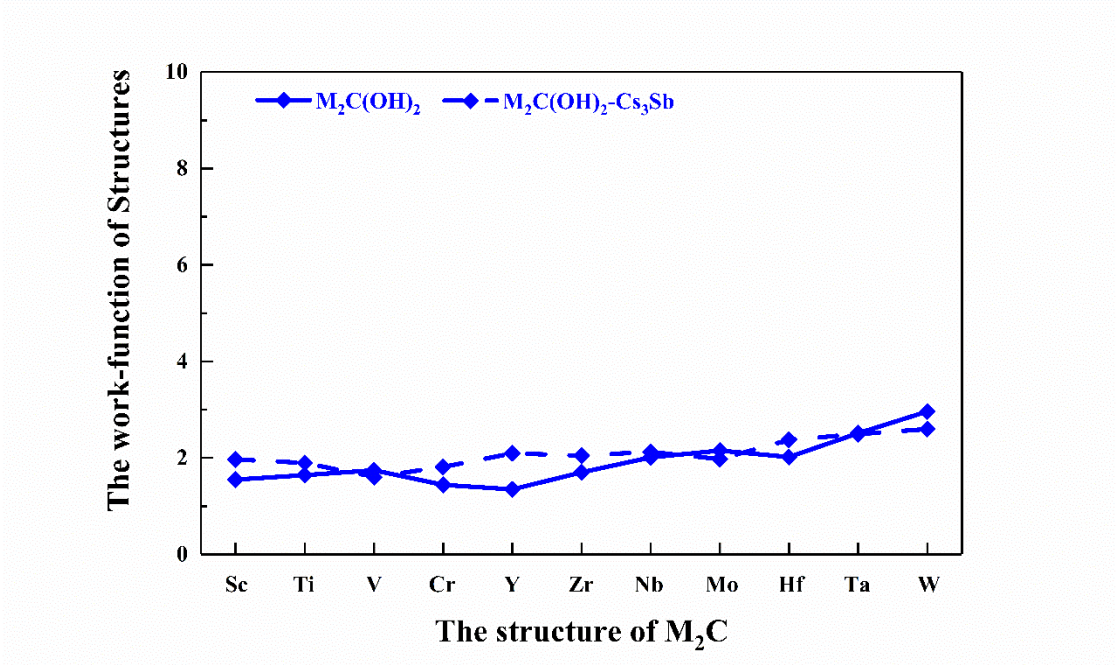


图 S3 $M_2C(OH)_2$/$M_2C(OH)_2$-Cs_3Sb结构的功函数随原子序数变化图

Fig. S3. Work-function of $M_2C(OH)_2$ and $M_2C(OH)_2$-Cs_3Sb structure vary with element number.

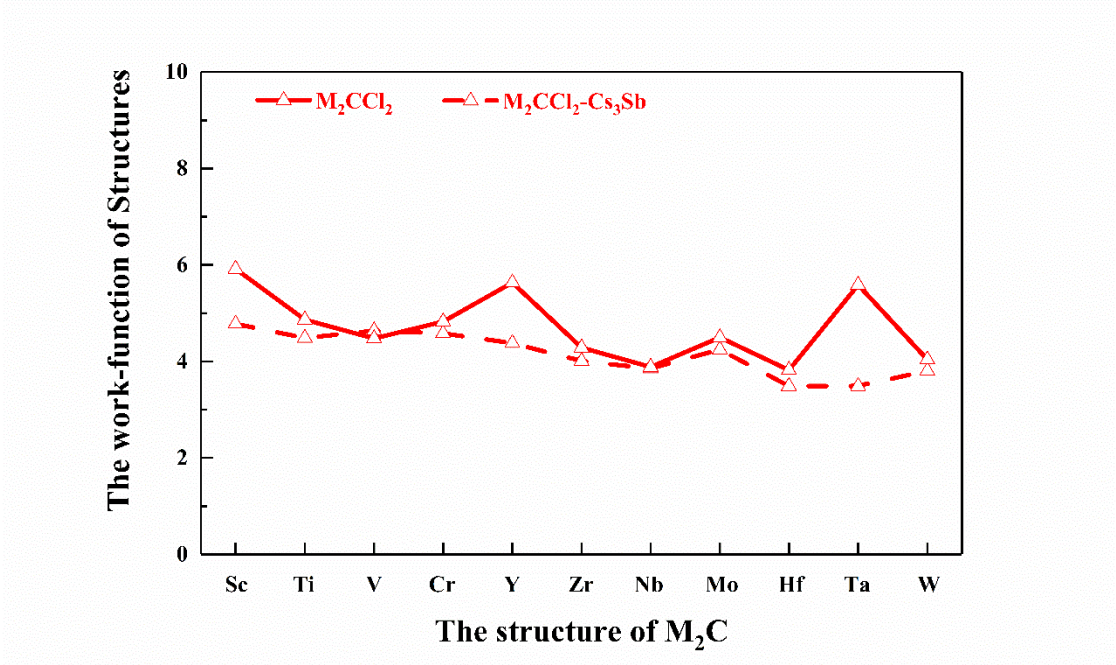


图 S4 M_2CCl_2/M_2CCl_2-Cs_3Sb结构的功函数随原子序数变化图

Fig. S4. Work-function of M_2CCl_2 and M_2CCl_2-Cs_3Sb structure vary with element number.

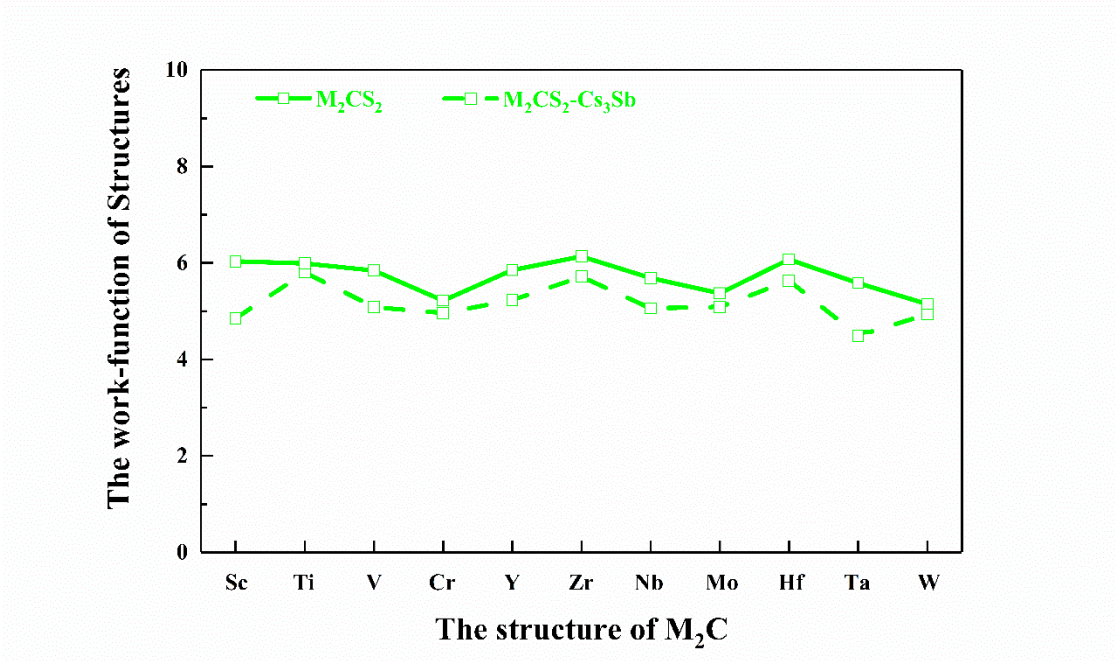


图 S5 M_2CS_2/M_2CS_2-Cs_3Sb结构的功函数随原子序数变化图

Fig. S5. Work-function of M_2CS_2 and M_2CS_2-Cs_3Sb structure vary with element number.

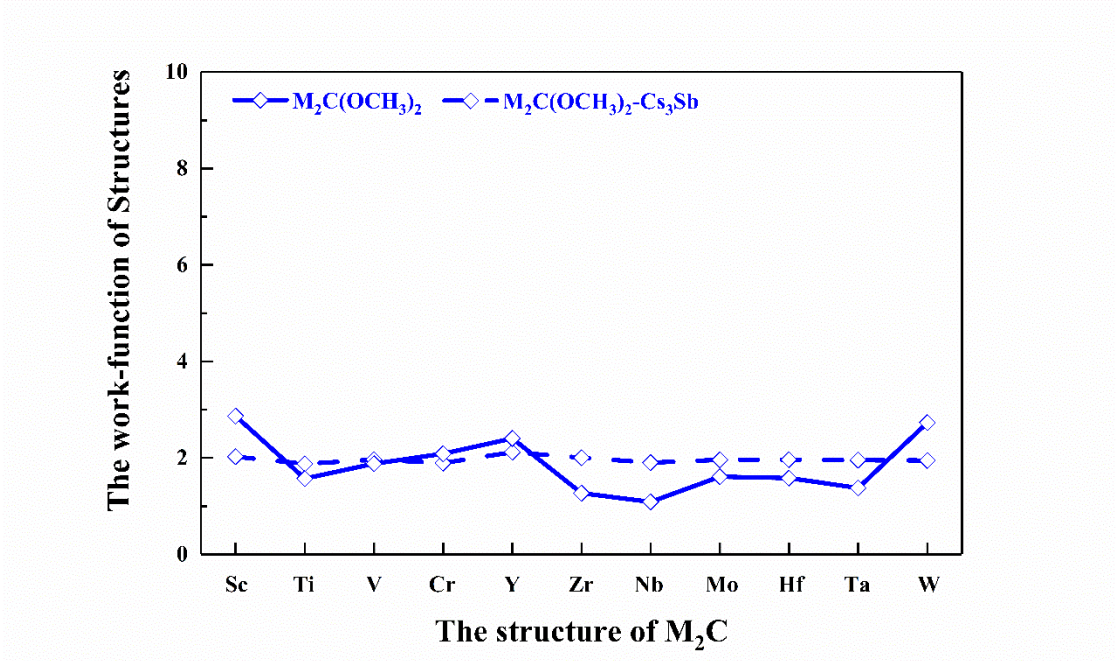


图 S6 $M_2C(OCH_3)_2$/$M_2C(OCH_3)_2$-Cs_3Sb结构的功函数随原子序数变化图

Fig. S6. Work-function of $M_2C(OCH_3)_2$ and $M_2C(OCH_3)_2$-Cs_3Sb structure vary with element number.

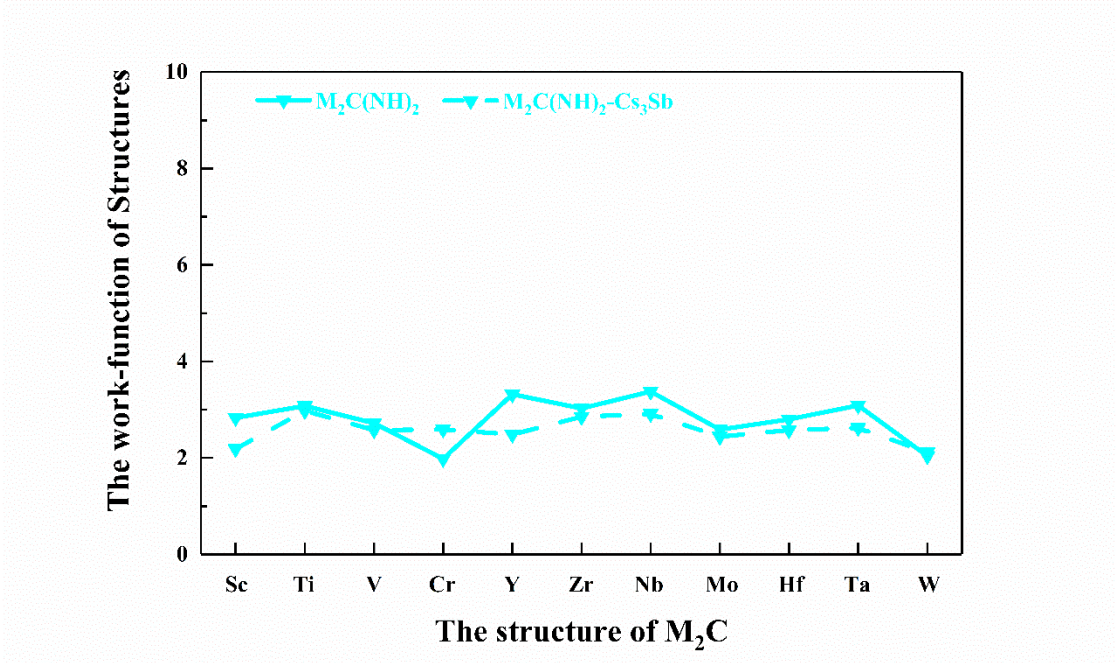


图 S7 $M_2C(NH)_2$/$M_2C(NH)_2$-Cs_3Sb结构的功函数随原子序数变化图

Fig. S7. Work-function of $M_2C(NH)_2$ and $M_2C(NH)_2$-Cs_3Sb structure vary with element number.

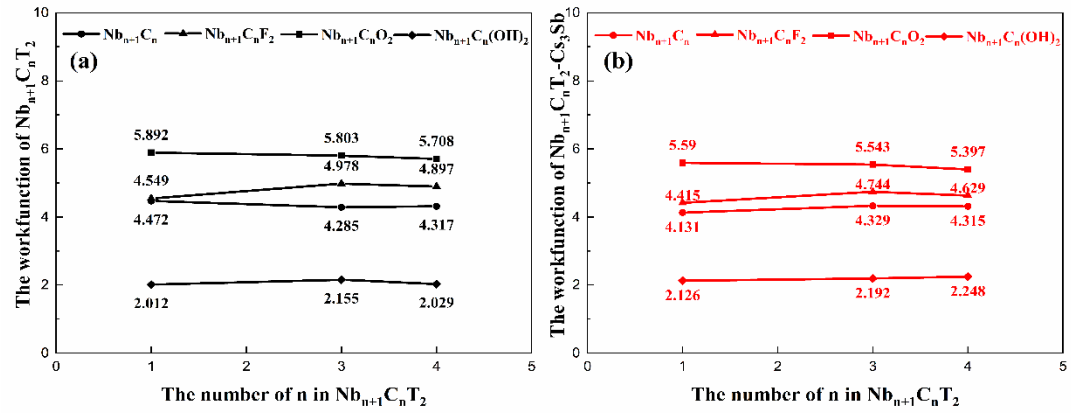


图 S8 $Nb_{n+1}C_nT_2$(n = 1, 3, 4)结构(a)和$Nb_{n+1}C_nT_2$-Cs_3Sb结构(b)的功函数随Nb/C原子比例变化图

Fig. S8. Work-function of $Nb_{n+1}C_nT_2$(n = 1, 3, 4) and $Nb_{n+1}C_nT_2$-Cs_3Sb structure vary with the ratio of Nb and C atom, shown in subgraph (a) and subgraph (b).

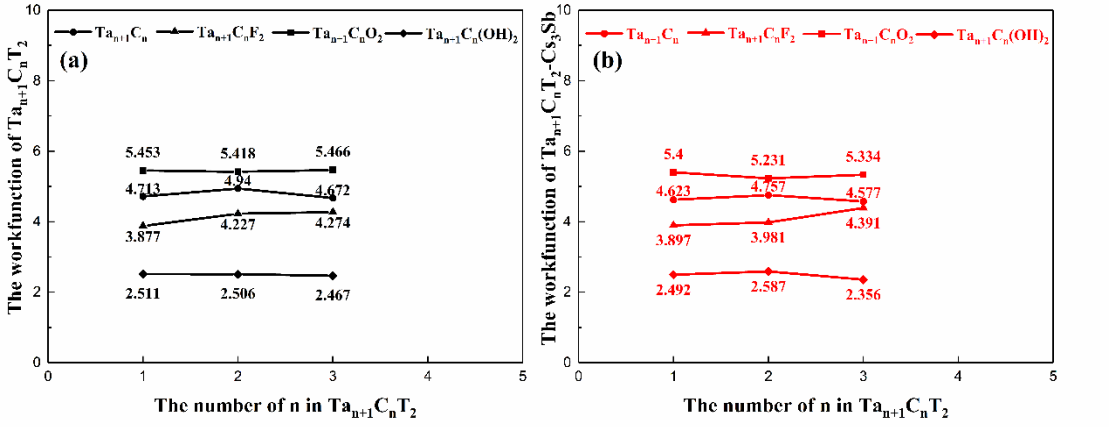


图 S9 $Ta_{n+1}C_nT_2$(n = 1, 2, 3)结构(a)和$Ta_{n+1}C_nT_2$-Cs_3Sb结构(b)的功函数随Ta/C原子比例变化图

Fig. S9. Work-function of $Ta_{n+1}C_nT_2$(n = 1, 2, 3) and $Ta_{n+1}C_nT_2$-Cs_3Sb structure vary with the ratio of Ta and C atom, shown in subgraph (a) and subgraph (b).

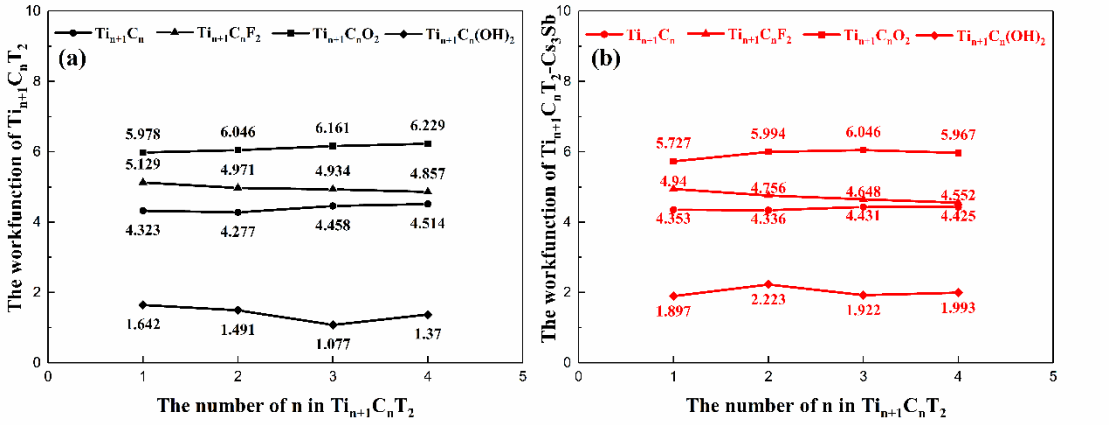


图 S10 $Ti_{n+1}C_nT_2$(n = 1, 2, 3, 4)结构(a)和$Ti_{n+1}C_nT_2$-Cs_3Sb结构(b)的功函数随Ti/C原子比例变化图

Fig. S10. Work-function of $Ti_{n+1}C_nT_2$ (n = 1, 2, 3, 4) and $Ti_{n+1}C_nT_2$-Cs_3Sb structure vary with the ratio of Ti and C atom, shown in subgraph (a) and subgraph (b).

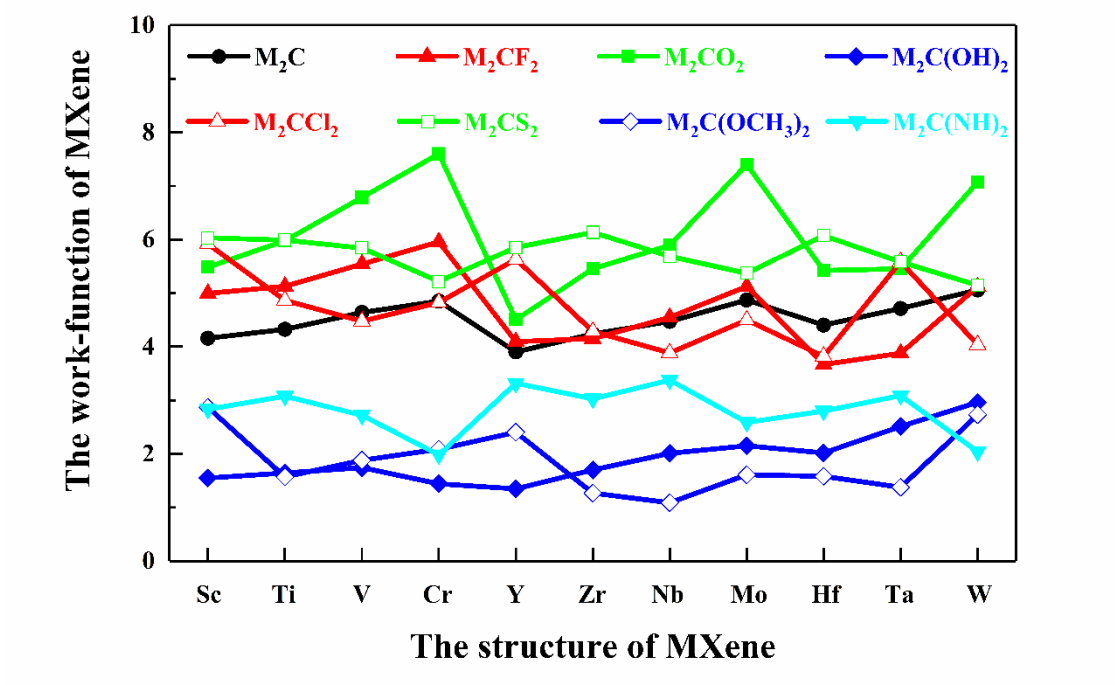


图 S11 M_2CT_2结构的功函数随M原子变化图。

Fig. S11. Work-function of M_2CT_2 structure vary with element number.

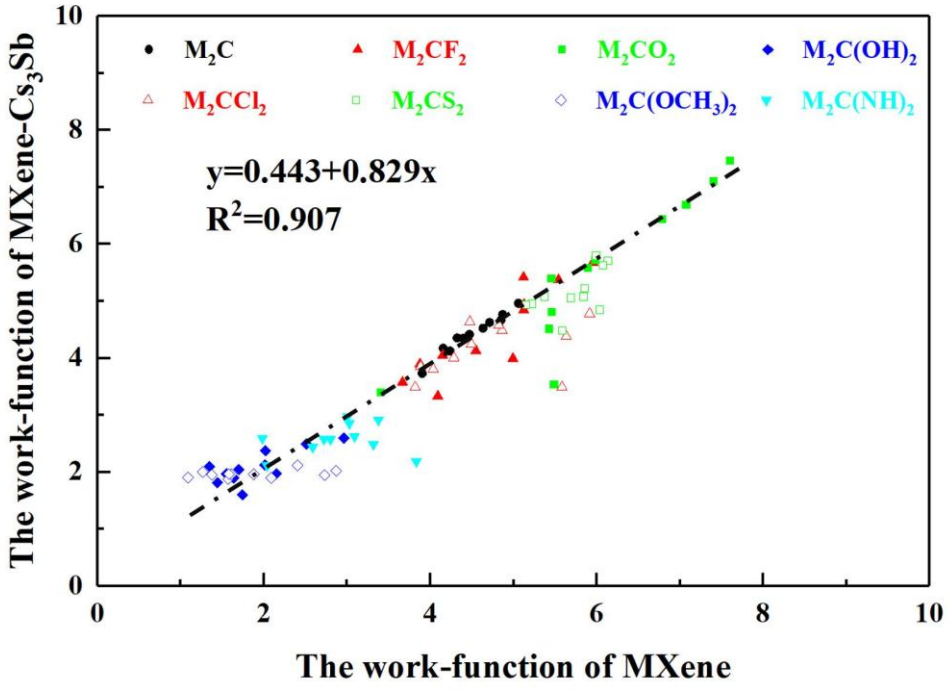


图 S12 M_2CT_2-Cs_3Sb结构的功函数随M_2CT_2结构功函数的变化图

Fig.S12. Relationship between the work-function of M_2CT_2-Cs_3Sb and the work-function (*W*) of M_2CT_2.

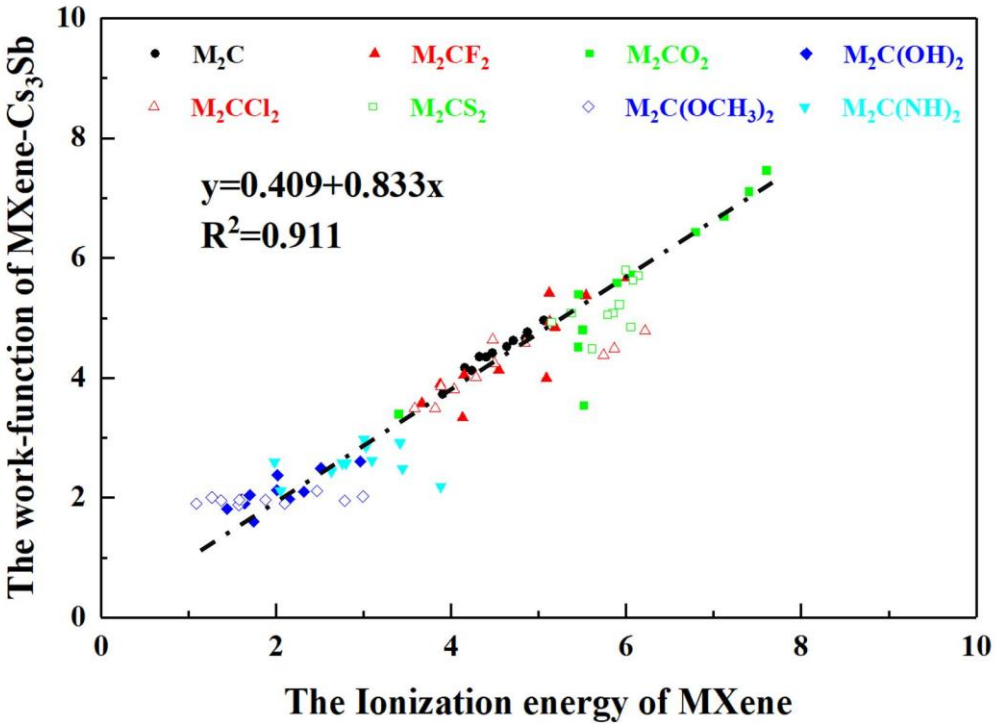
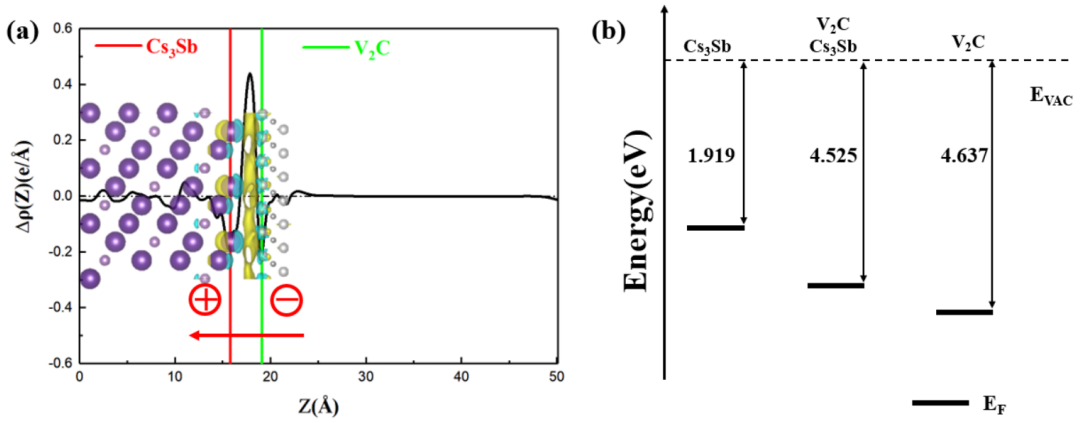


图 S13 M_2CT_2-Cs_3Sb结构的功函数随M_2CT_2结构的电离能(IP)变化图

Fig.S13. Relationship between the work-function of M_2CT_2-Cs_3Sb and the ionization energy (IP) of M_2CT_2.



图S 14 V_2C-Cs_3Sb异质结的差分电荷密度图(a)和能级校正分析示意图(b)，等值面设为0.001 *e*/bohr^3

Figure. S14. Charge density difference and band alignment of V_2C-Cs_3Sb structures, shown in subgraph (a) and (b), the isosurface value is set to 0.001 *e*/bohr^3.

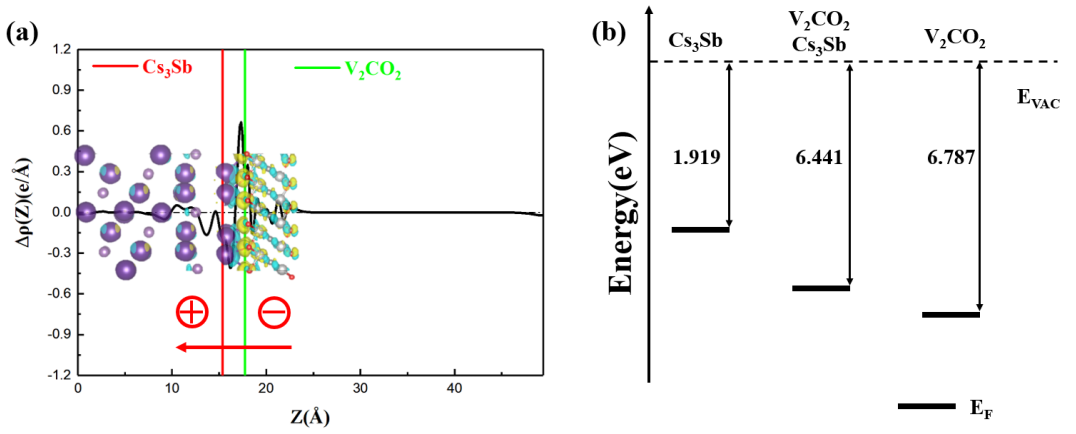


图 S15 V_2CO_2-Cs_3Sb异质结的差分电荷密度图(a)和能级校正分析示意图(b)，等值面设为 0.003 *e*/bohr^3

Figure. S15. Charge density difference and band alignment of V_2CO_2-Cs_3Sb structures, shown in subgraph (a) and (b), the isosurface value is set to 0.003 *e*/bohr^3.

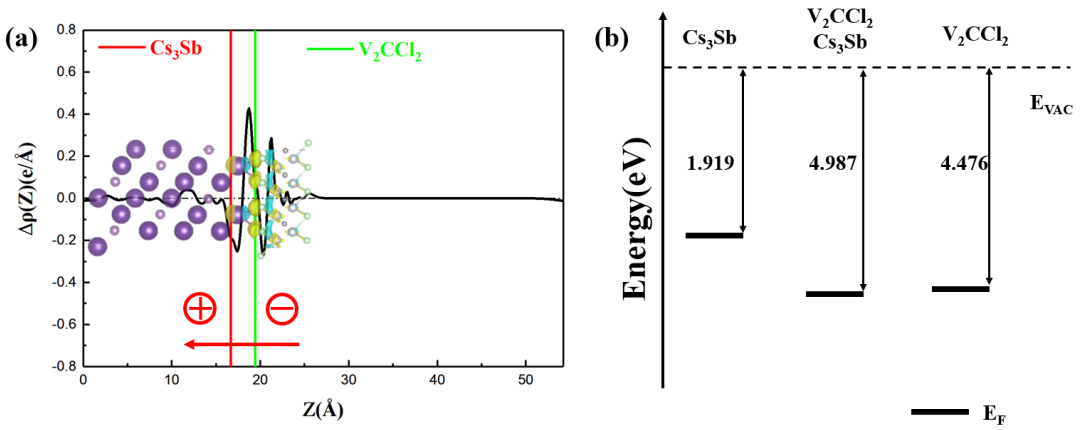
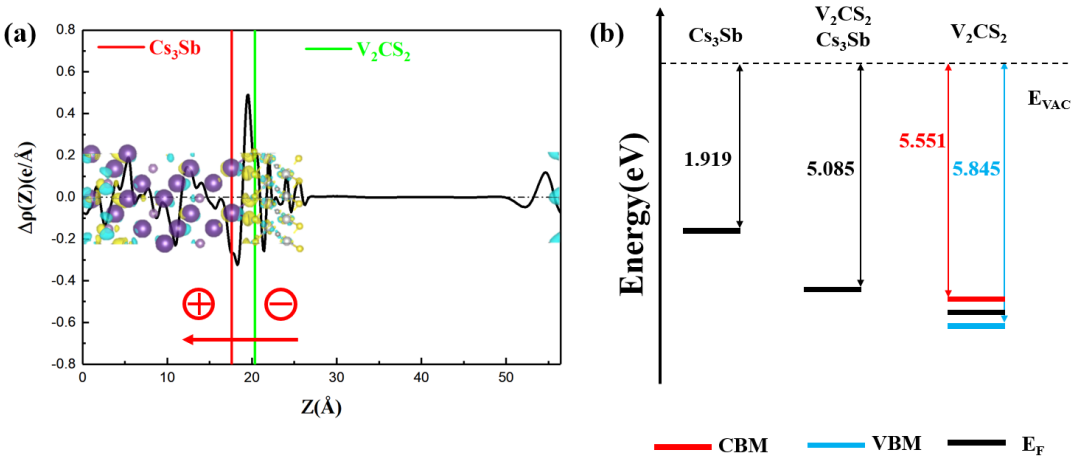


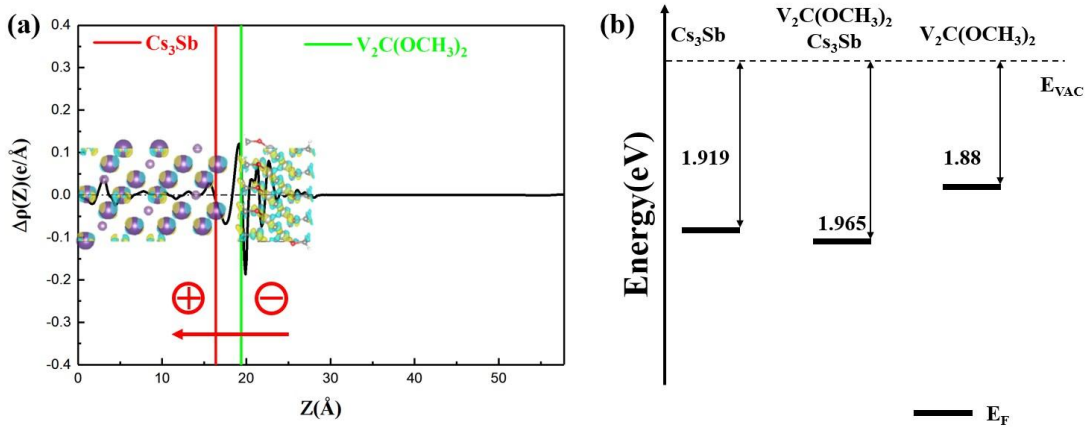
图 S16 V_2CCl_2-Cs_3Sb异质结的差分电荷密度图(a)和能级校正分析示意图(b)，等值面设为 0.001 *e*/bohr^3

Figure. S16. Charge density difference and band alignment of V_2CCl_2-Cs_3Sb structures, shown in subgraph (a) and (b), the isosurface value is set to 0.001*e*/bohr^3.



图S 17 V_2CS_2-Cs_3Sb异质结的差分电荷密度图(a)和能级校正分析示意图(b)，等值面设为0.0015 *e*/bohr^3

Figure. S17. Charge density difference and band alignment of V_2CS_2-Cs_3Sb structures, shown in subgraph (a) and (b)， the isosurface value is set to 0.0015 *e*/bohr^3.



图S 18 $V_2C(OCH_3)_2$-Cs_3Sb异质结的差分电荷密度图(a)和能级校正分析示意图(b)，等值面设为0.002 *e*/bohr^3

Figure. S18. Charge density difference and band alignment of $V_2C(OCH_3)_2$-Cs_3Sb structures, shown in subgraph (a) and (b), the isosurface value is set to 0.002 *e*/bohr^3.

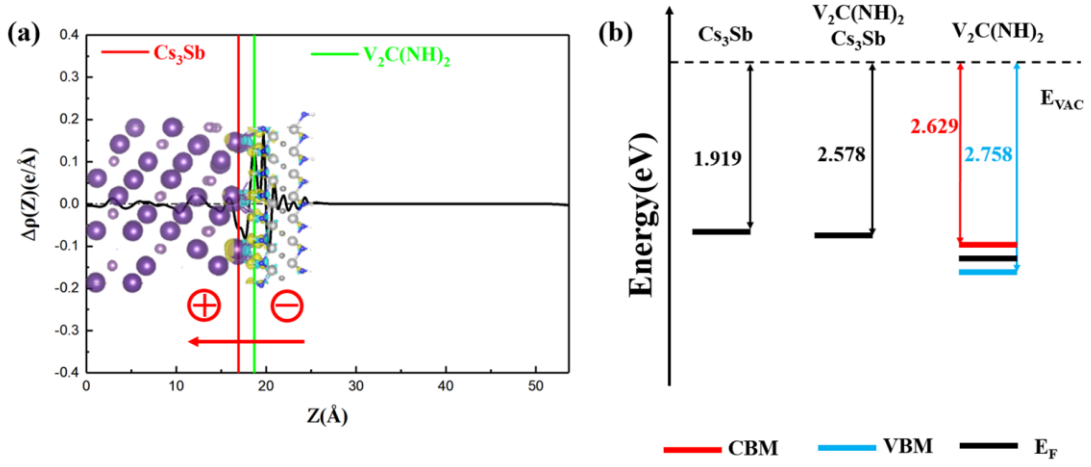


图 S19 $V_2C(NH)_2$-Cs_3Sb异质结的差分电荷密度图(a)和能级校正分析示意图(b)，等值面设为 0.0015 *e*/bohr^3

Figure. S19. Charge density difference and band alignment of $V_2C(NH)_2$-Cs_3Sb structures, shown in subgraph (a) and (b), the isosurface value is set to 0.0015 *e*/bohr^3.