

补充材料

基于 MXene 涂层保护 Cs₃Sb 异质结光阴极材料的计算筛选*

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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 $0.0015 e/bohr^3$)。

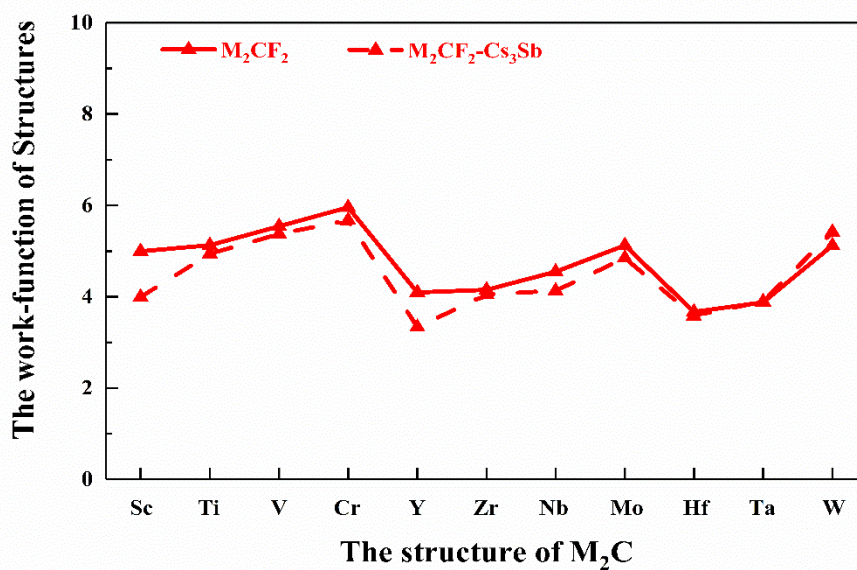


图 S1 $M_2CF_2/M_2CF_2-Cs_3Sb$ 结构的功函数随原子序数变化图

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

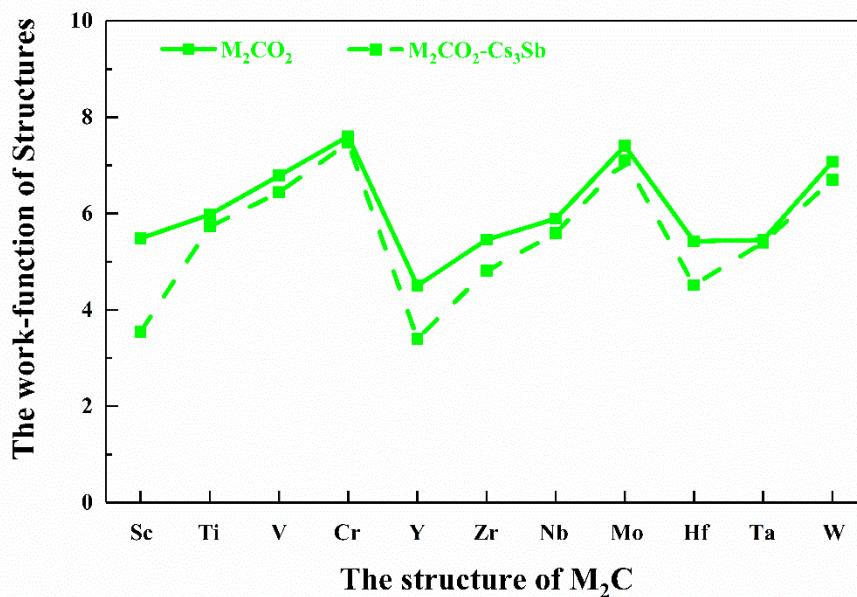


图 S2 $M_2CO_2/M_2CO_2-Cs_3Sb$ 结构的功函数随原子序数变化图

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

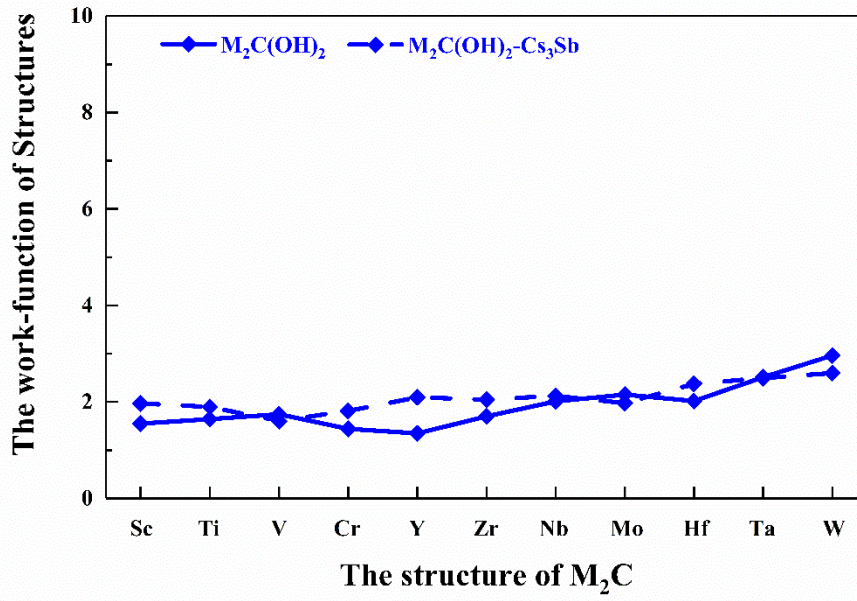


图 S3 M₂C(OH)₂/M₂C(OH)₂-Cs₃Sb结构的功函数随原子序数变化图

Fig. S3. Work-function of M₂C(OH)₂ and M₂C(OH)₂-Cs₃Sb structure vary with element number.

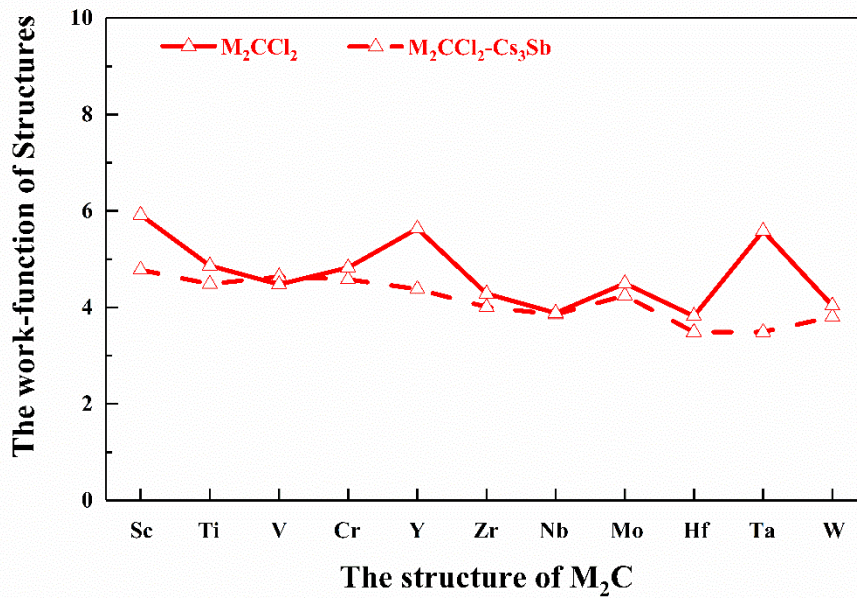


图 S4 M₂CCl₂/M₂CCl₂-Cs₃Sb结构的功函数随原子序数变化图

Fig. S4. Work-function of M₂CCl₂ and M₂CCl₂-Cs₃Sb structure vary with element number.

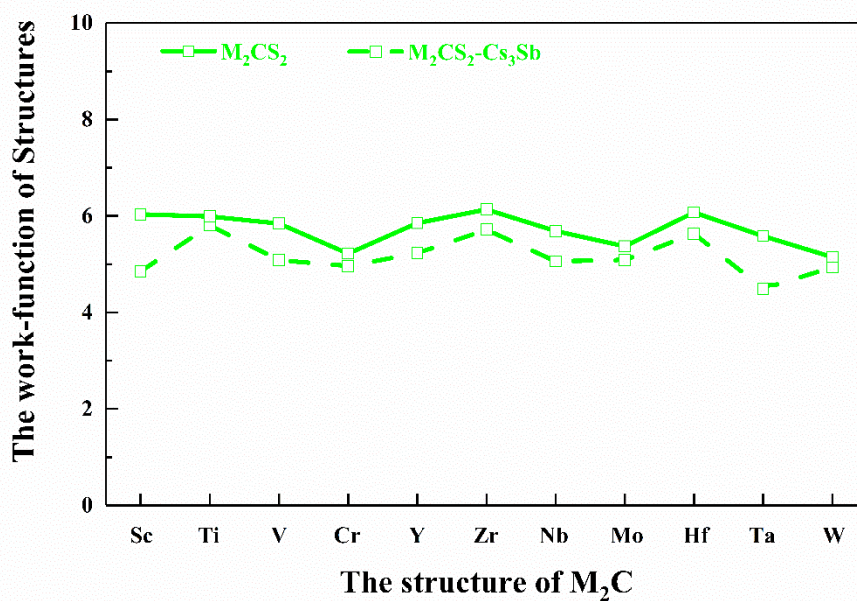


图 S5 $M_2CS_2/M_2CS_2-Cs_3Sb$ 结构的功函数随原子序数变化图

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

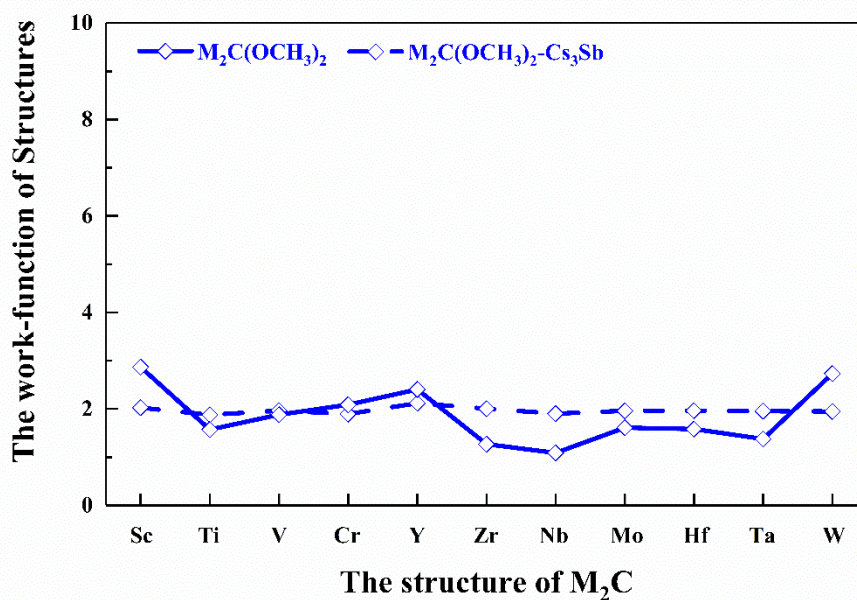


图 S6 $M_2C(OCH_3)_2/M_2C(OCH_3)_2-Cs_3Sb$ 结构的功函数随原子序数变化图

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

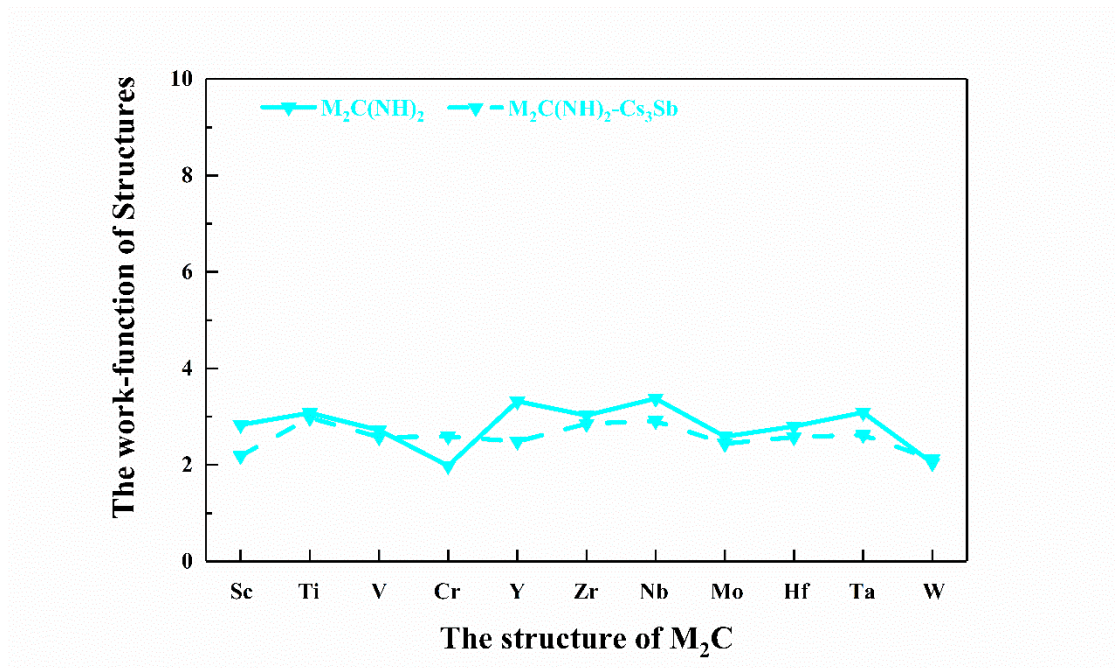


图 S7 $M_2C(NH)_2/M_2C(NH)_2-Cs_3Sb$ 结构的功函数随原子序数变化图

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

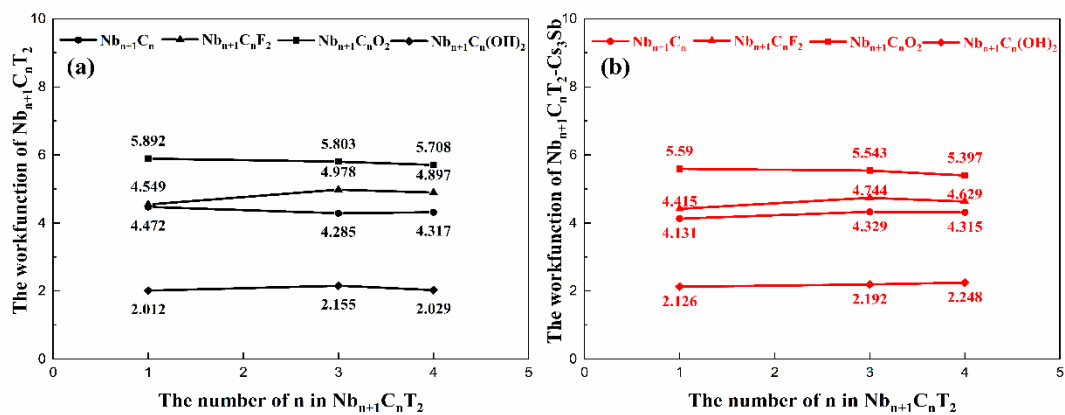


图 S8 $Nb_{n+1}C_nT_2$ ($n = 1, 3, 4$) 结构(a)和 $Nb_{n+1}C_nT_2-Cs_3Sb$ 结构(b)的功函数随Nb/C原子比例变化

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).

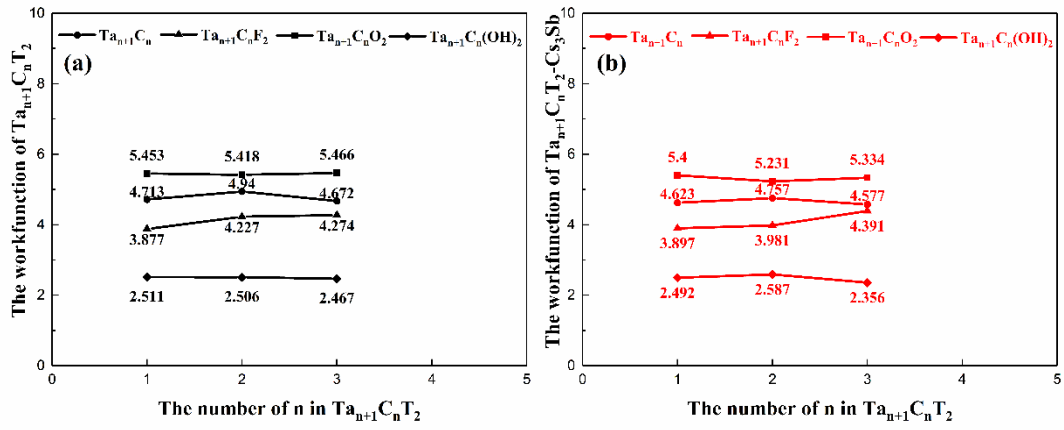


图 S9 Ta_{n+1}C_nT₂(n = 1, 2, 3)结构(a)和Ta_{n+1}C_nT₂-Cs₃Sb结构(b)的功函数随Ta/C原子比例变化图

Fig. S9. Work-function of Ta_{n+1}C_nT₂(n = 1, 2, 3) and Ta_{n+1}C_nT₂-Cs₃Sb structure vary with the ratio of Ta and C atom, shown in subgraph (a) and subgraph (b).

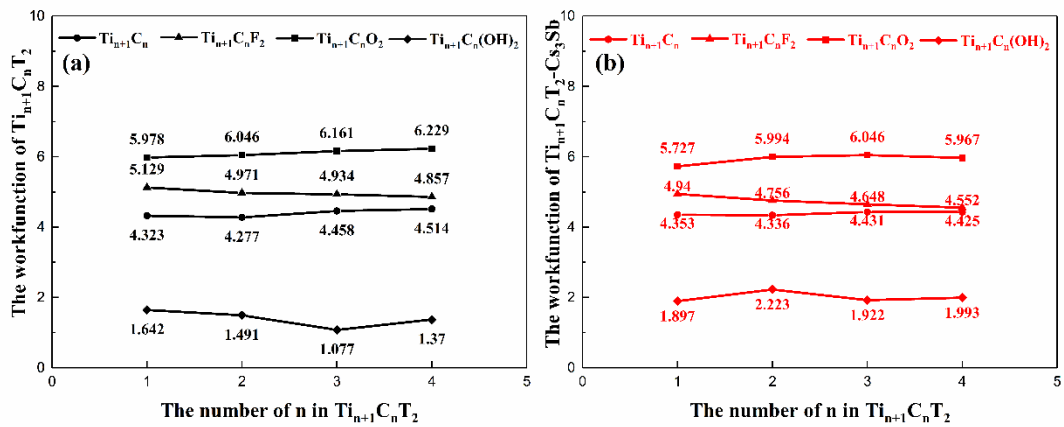


图 S10 Ti_{n+1}C_nT₂(n = 1, 2, 3, 4)结构(a)和Ti_{n+1}C_nT₂-Cs₃Sb结构(b)的功函数随Ti/C原子比例变化

图

Fig. S10. Work-function of Ti_{n+1}C_nT₂ (n = 1, 2, 3, 4) and Ti_{n+1}C_nT₂-Cs₃Sb structure vary with the ratio of Ti and C atom, shown in subgraph (a) and subgraph (b).

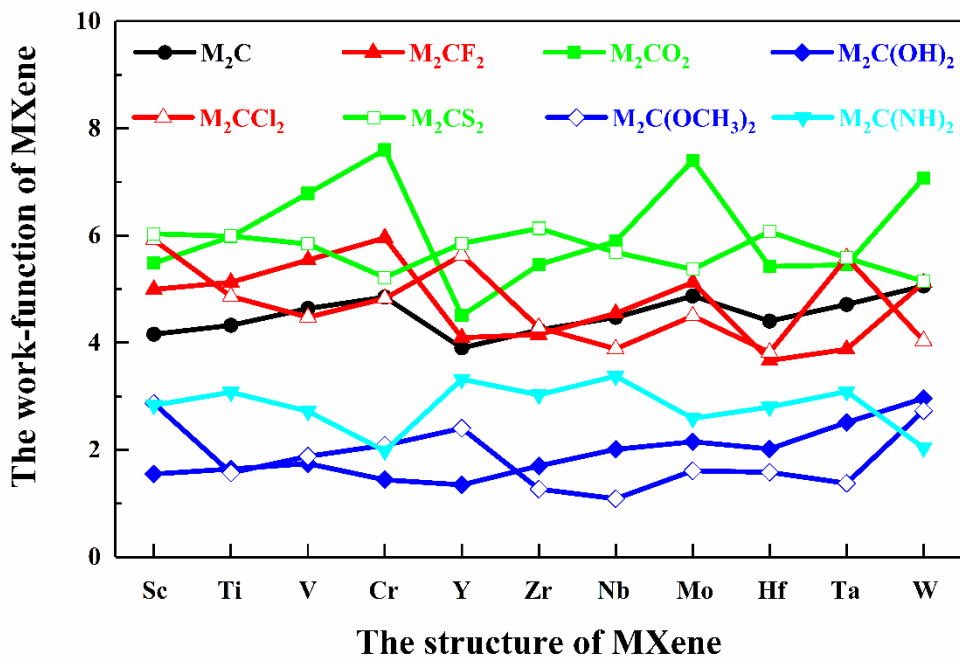


图 S11 M_2CT_2 结构的功函数随M原子变化图。

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

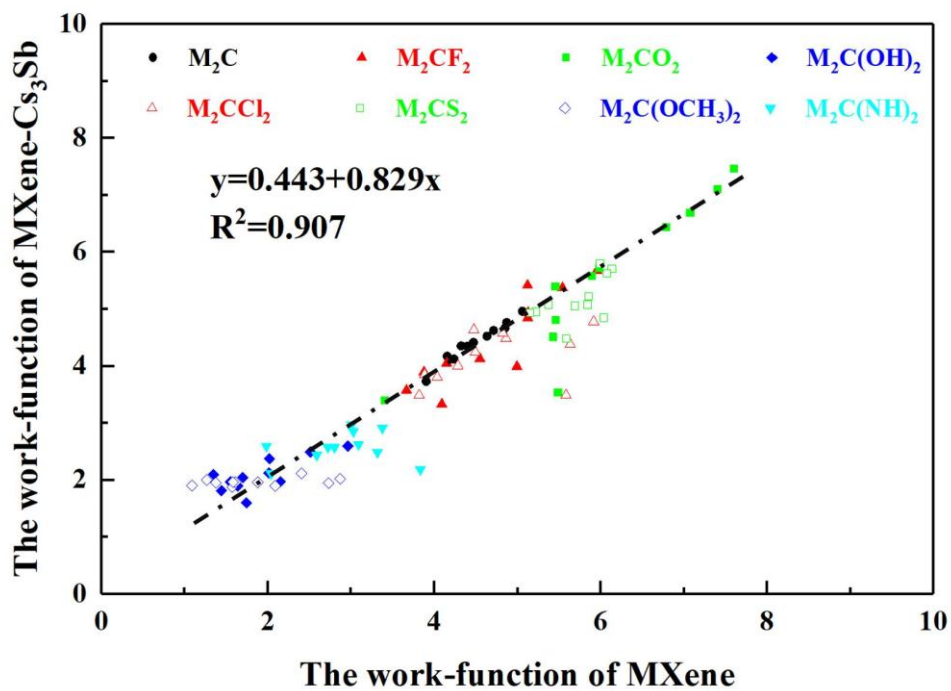


图 S12 M_2CT_2 - Cs_3Sb 结构的功函数随 M_2CT_2 结构功函数的变化图

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

M_2CT_2 .

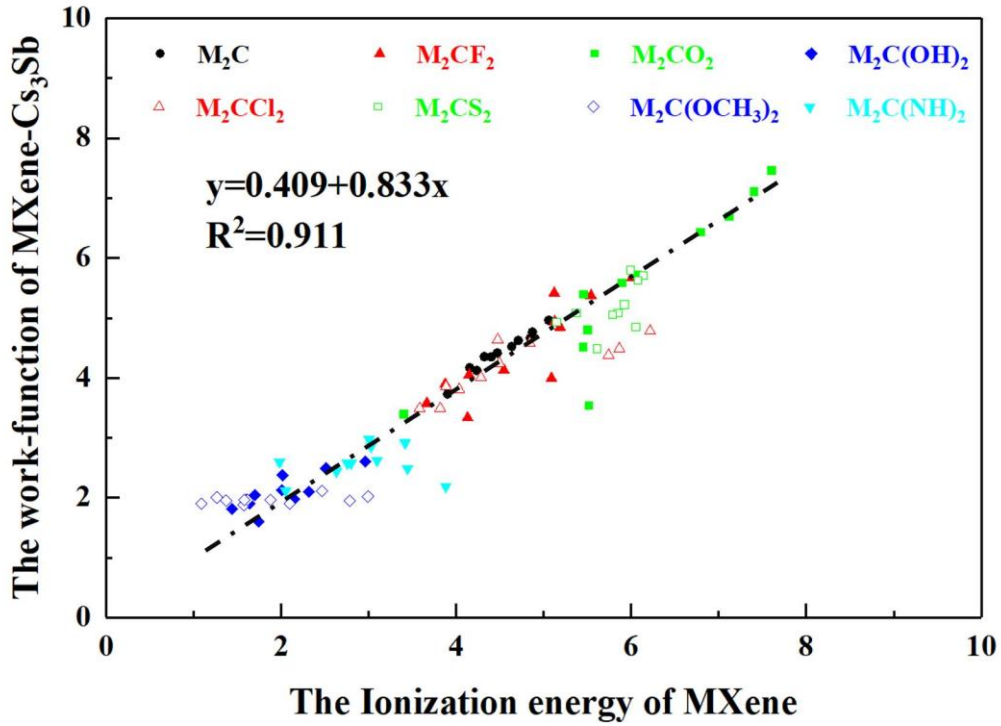
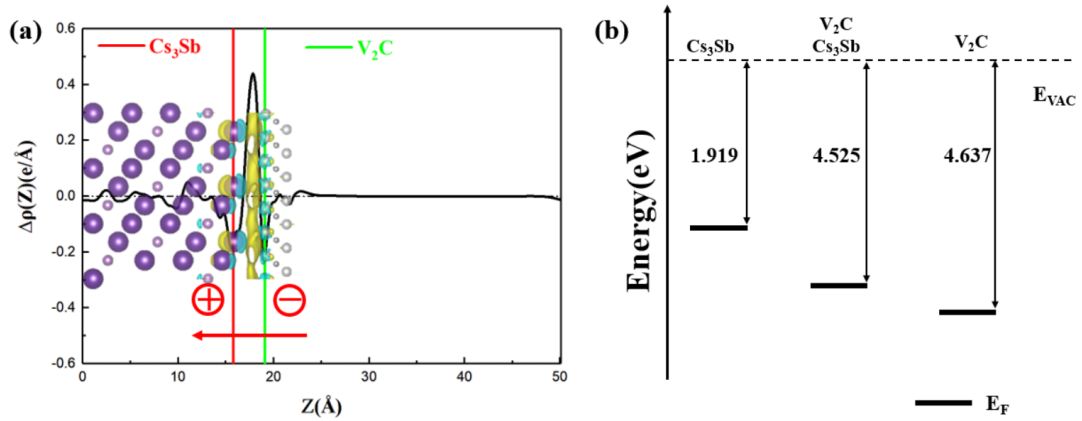


图 S13 M_2CT_2 - Cs_3Sb 结构的功函数随 M_2CT_2 结构的电离能(IP)变化图

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 $0.001 e/\text{bohr}^3$.

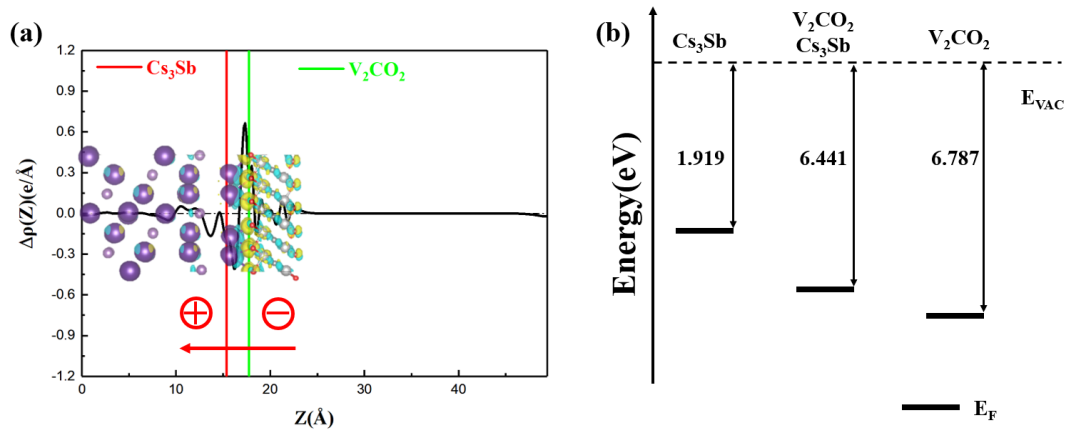


图 S15 V_2CO_2 - Cs_3Sb 异质结的差分电荷密度图(a)和能级校正分析示意图(b), 等值面设为

$0.003 e/\text{bohr}^3$

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 $0.003 e/\text{bohr}^3$.

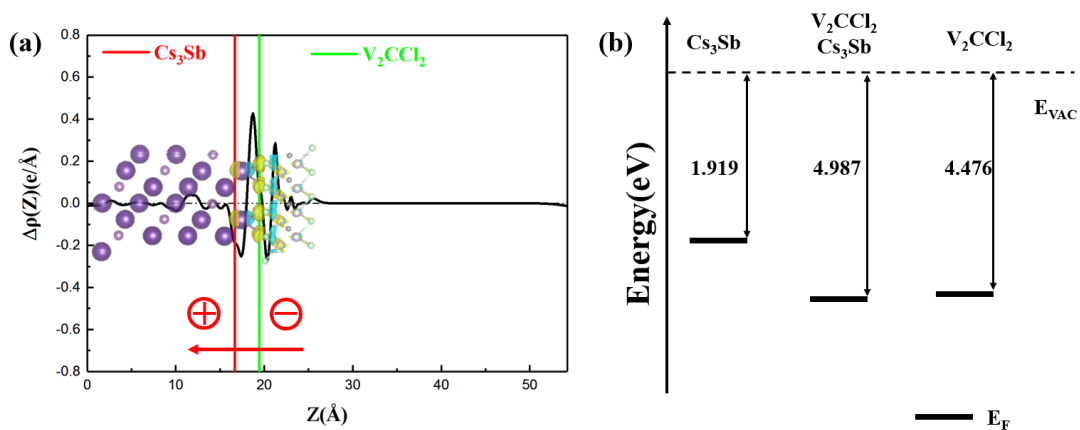
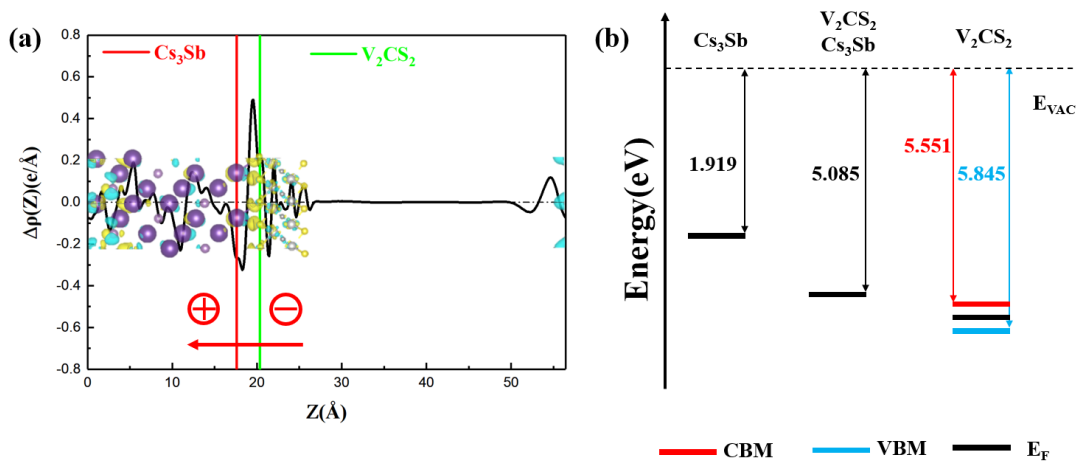


图 S16 V_2CCl_2 - Cs_3Sb 异质结的差分电荷密度图(a)和能级校正分析示意图(b), 等值面设为

$0.001 e/\text{bohr}^3$

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 $0.001 e/\text{bohr}^3$.

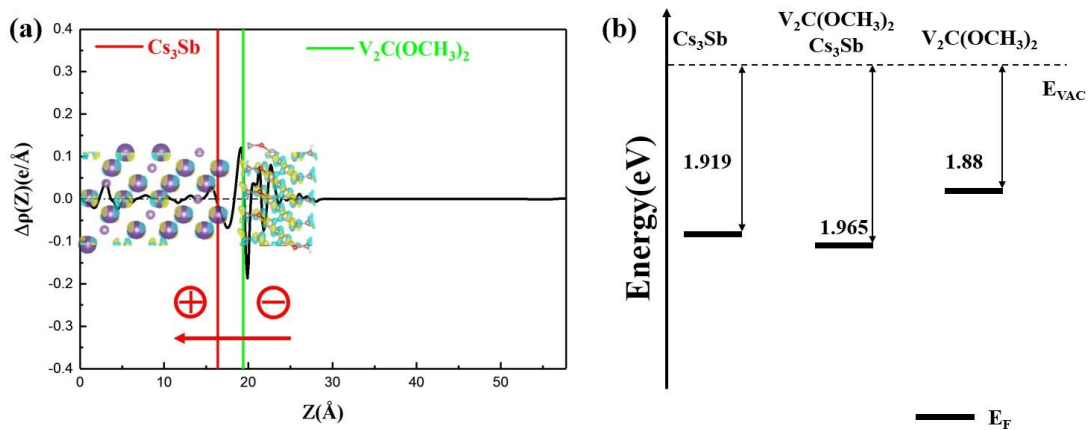


图S 17 V_2CS_2 - Cs_3Sb 异质结的差分电荷密度图(a)和能级校正分析示意图(b)，等值面设为

$0.0015 e/\text{bohr}^3$

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 $0.0015 e/\text{bohr}^3$.



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 $0.002 e/\text{bohr}^3$

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 $0.002 e/\text{bohr}^3$.

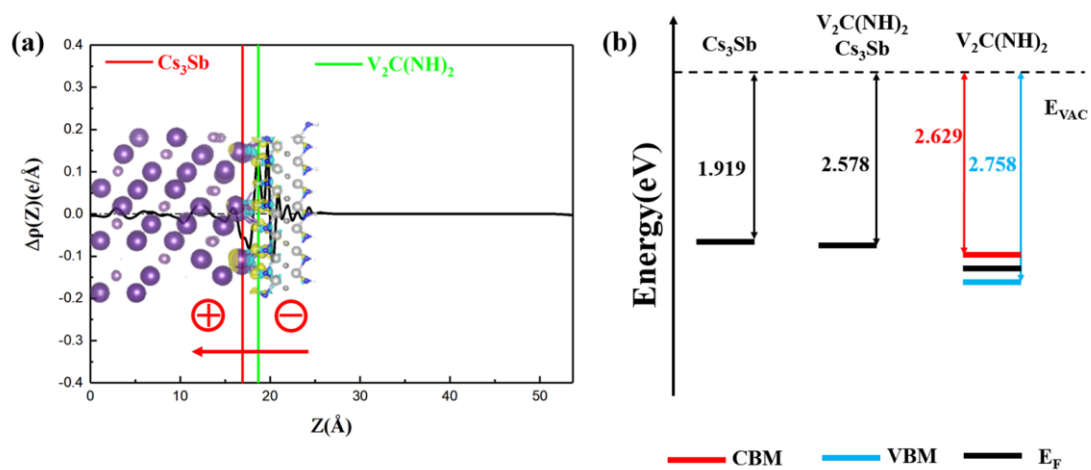


图 S19 $\text{V}_2\text{C}(\text{NH})_2\text{-Cs}_3\text{Sb}$ 异质结的差分电荷密度图(a)和能级校正分析示意图(b), 等值面设为

$$0.0015 e/\text{bohr}^3$$

Figure. S19. Charge density difference and band alignment of $\text{V}_2\text{C}(\text{NH})_2\text{-Cs}_3\text{Sb}$ structures, shown

in subgraph (a) and (b), the isosurface value is set to $0.0015 e/\text{bohr}^3$.