Supporting information for

Modified MXene: Promising electrode materials for constructing Ohmic contact with MoS$_2$ for electronic device application

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Figure S1. Side views of six different stacking patterns of MoS$_2$/Ta$_2$CY$_2$(Y=F, OH) structures. The yellow, purple, green, white, red, orange and black balls are S, Mo, F, H, O, Ta and C atoms respectively.

Figure S2. The scatter diagram of binding energy for MoS$_2$/Ta$_2$C, MoS$_2$/Ta$_2$CF$_2$ and MoS$_2$/Ta$_2$C(OH)$_2$ systems respectively.

Figure S3. The charge difference between MoS$_2$ and (a)Ta$_2$C, (b) Ta$_2$CF$_2$, (c)Ta$_2$C(OH)$_2$. The yellow and green region represent electron accumulation and depletion, respectively.
Figure S4. Partial density of states (PDOS) of pure monolayer MoS\textsubscript{2} on the Ta\textsubscript{2}C, Ta\textsubscript{2}CF\textsubscript{2} and Ta\textsubscript{2}C(OH)\textsubscript{2}. The fermi level is set at zero energy.

Figure S5. The electron localization function (ELF) of (a) MoS\textsubscript{2}/Ta\textsubscript{2}C, (b) MoS\textsubscript{2}/Ta\textsubscript{2}CF\textsubscript{2} and (c) MoS\textsubscript{2}/Ta\textsubscript{2}C(OH)\textsubscript{2} systems.