Supporting information for

Modified MXene : Promising electrode materials for constructing Ohmic contact with MoS_2 for electronic device application

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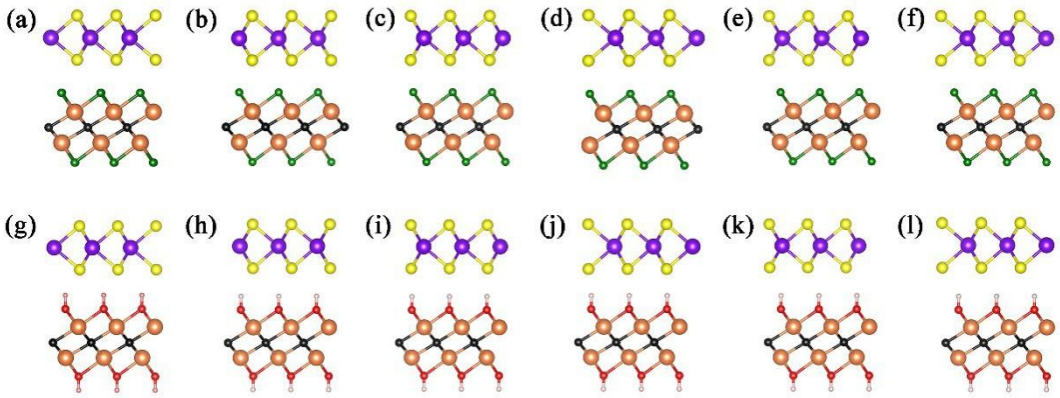

Figure S1. Side views of six different stacking patterns of MoS_2/Ta_2CY_2(Y=F, OH) structures. The yellow, purples, green, white, red, orange and black balls are S, Mo, F, H, O, Ta and C atoms respectively.

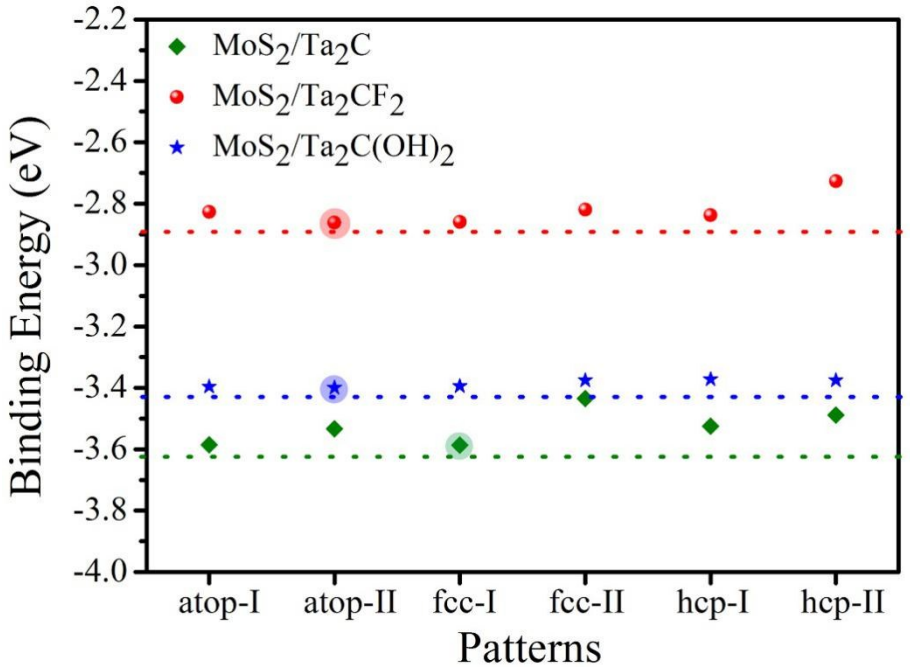

Figure S2. The scatter diagram of binding energy for MoS_2/Ta_2C, MoS_2/Ta_2CF_2 and $MoS_2/Ta_2C(OH)_2$ systems respectively.

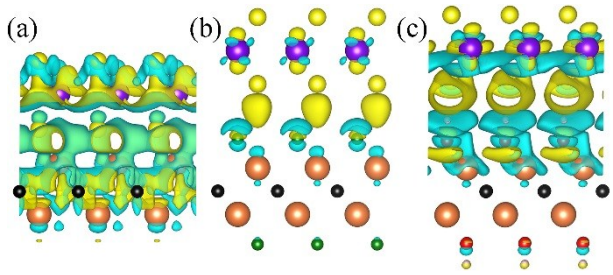

Figure S3. The charge difference between MoS_2 and (a)Ta_2C, (b) Ta_2CF_2, (c)$Ta_2C(OH)_2$. The yellow and green region represent electron accumulation and depletion, respectively.

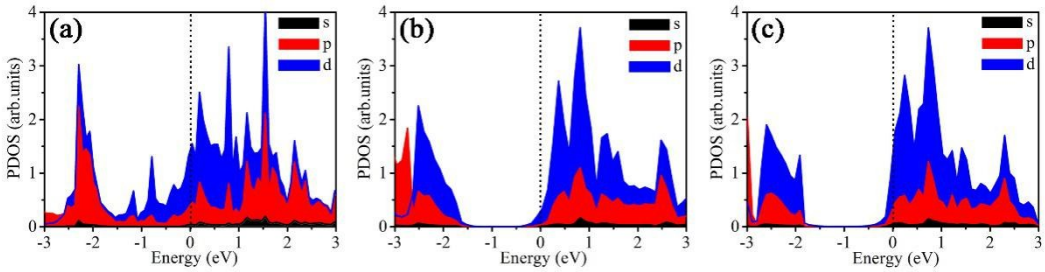

Figure S4. Partial density of states (PDOS) of pure monolayer MoS_2 on the Ta_2C, Ta_2CF_2 and $Ta_2C(OH)_2$. The fermi level is set at zero energy.

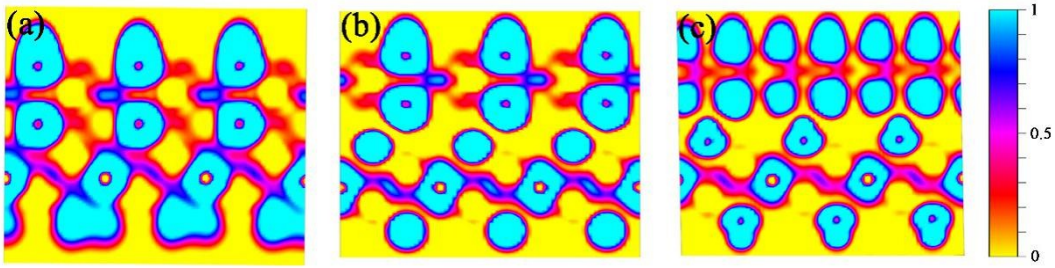

Figure S5. The electron localization function (ELF) of (a) MoS_2/Ta_2C, (b) MoS_2/Ta_2CF_2 and (c) $MoS_2/Ta_2C(OH)_2$ systems.