Electronic supplementary information (ESI)

Tuning Electronic and Optical Properties of MoS_2 Monolayer via Molecular Charge Transfer

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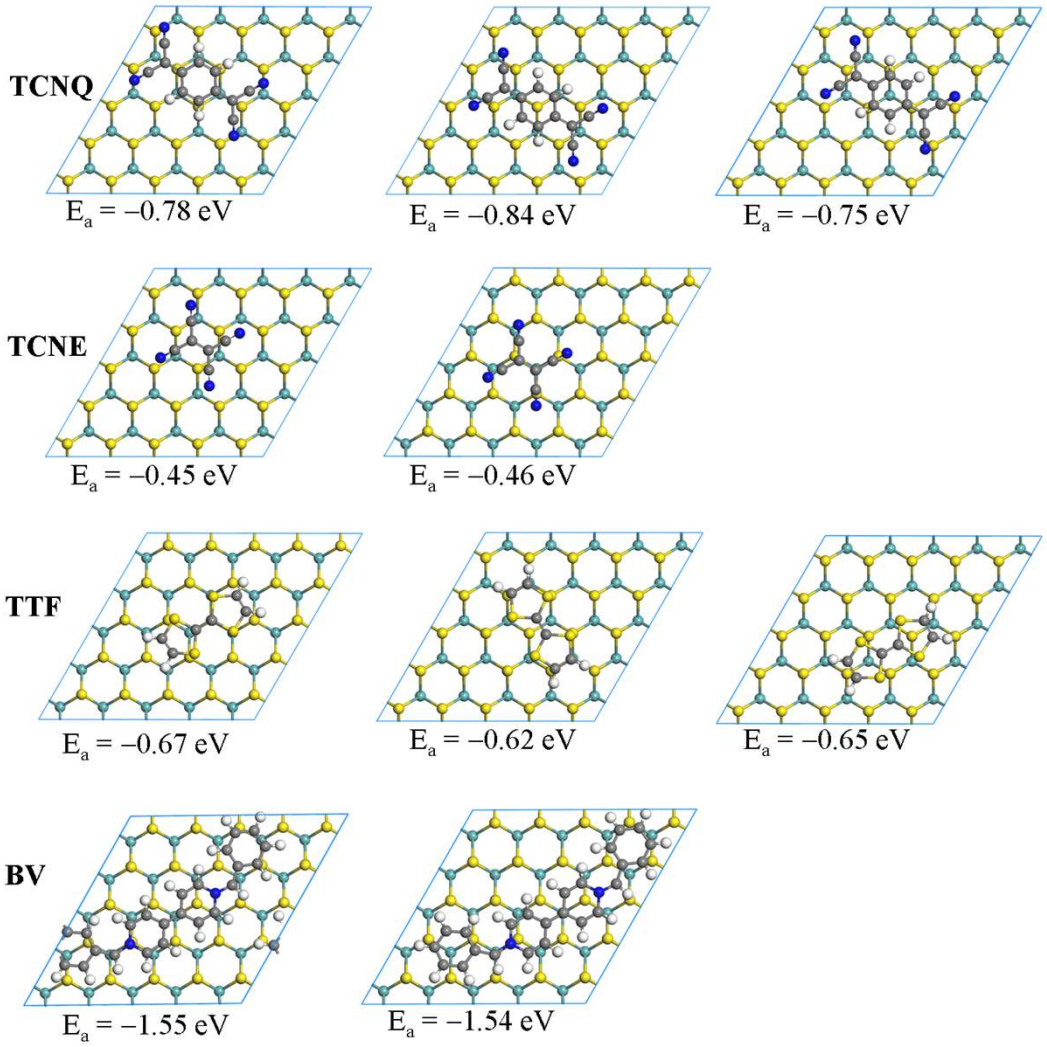

Figure S1. The optimized structures and corresponding adsorption energies of all the possible configurations for the adsorption of TCNQ, TCNE, TTF and BV molecules on the basal plane of MoS_2ML.

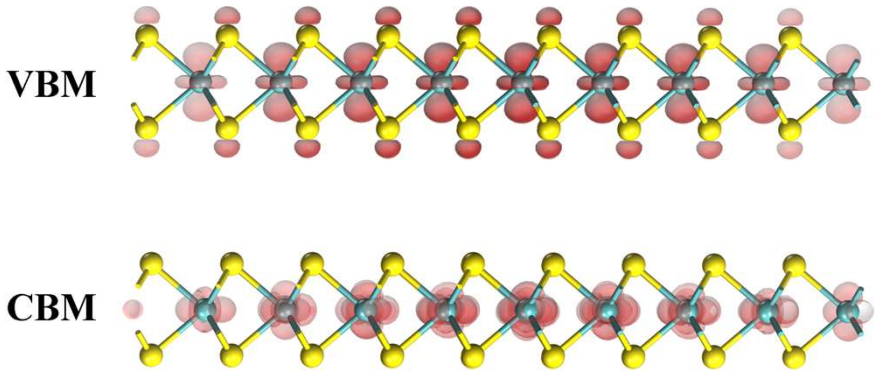

Figure S2. The partial charge density for the CBM and VBM of MoS_2ML.

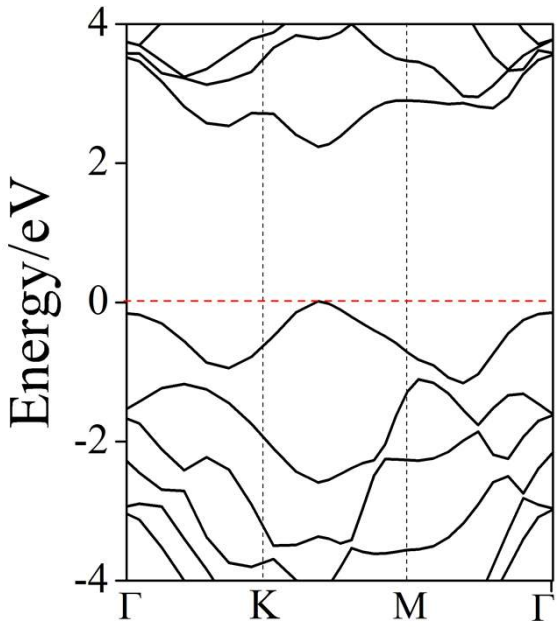

Figure S3. Band structure of MoS_2ML computed by using HSE06 functional.

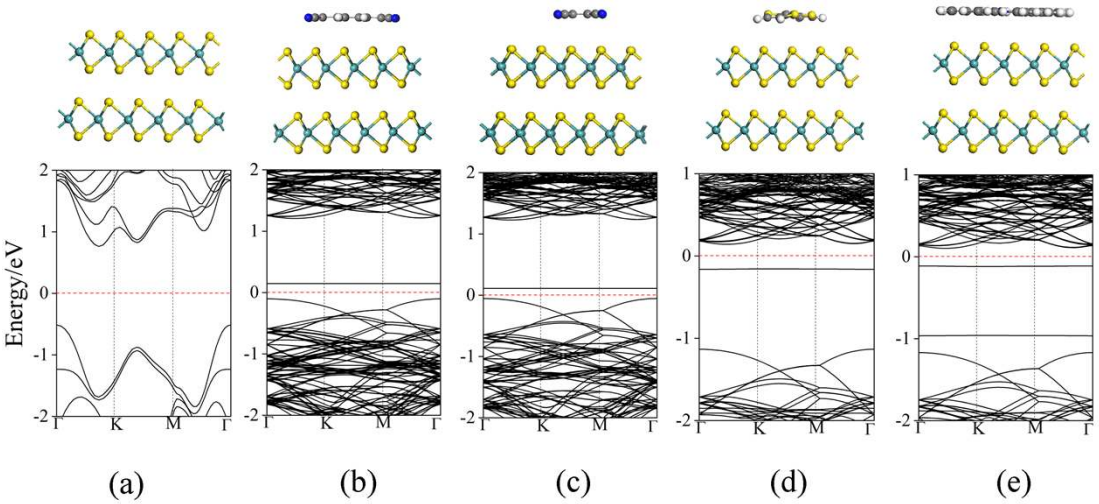

Figure S4. Geometric structures (upper) and band structures (bottom) of free-standing MoS_2BL (a) as well as those functionalized with TCNQ (b), TCNE (c), TTF (d), and BV (d).