

Electronic supplementary information (ESI)

Tuning Electronic and Optical Properties of MoS₂ Monolayer via Molecular Charge Transfer

Yu Jing,[†] Xin Tan,[‡] Zhen Zhou^{†,*} and Panwen Shen[†]

Tianjin Key Laboratory of Metal and Molecule Based Material Chemistry, Key Laboratory of Advanced Energy Materials Chemistry (Ministry of Education), Computational Centre for Molecular Science, Institute of New Energy Material Chemistry, Collaborative Innovation Center of Chemical Science and Engineering (Tianjin), Nankai University, Tianjin 300071, P. R. China; and School of Materials, Optoelectronics and Physics, Xiangtan University, Xiangtan 411105, Hunan, P. R. China

[†] Nankai University

[‡] Xiangtan University

* To whom correspondence should be addressed. Email: zhouzhen@nankai.edu.cn

(Z.Z.)

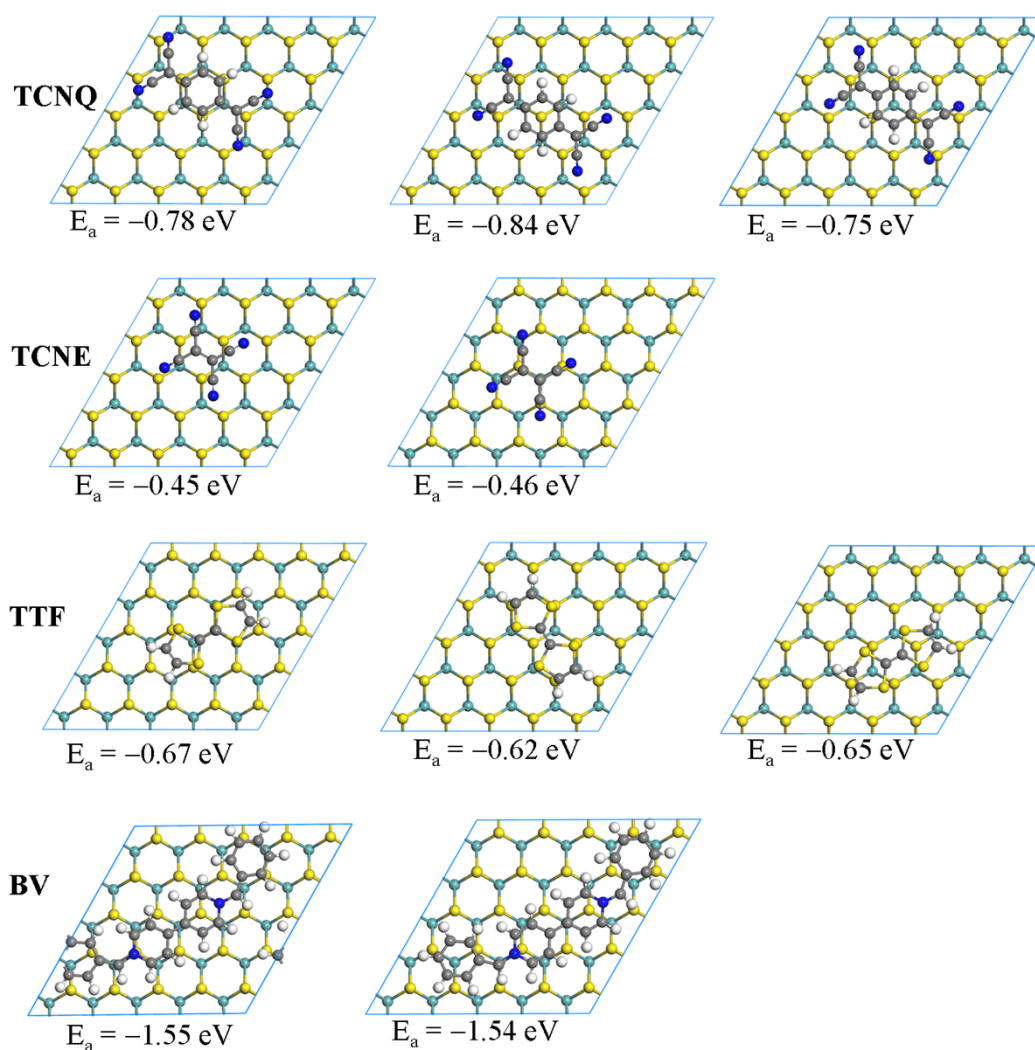


Figure S1. The optimized structures and corresponding adsorption energies of all the possible configurations for the adsorption of TCNQ, TCNE, TTF and BV molecules on the basal plane of MoS₂ML.

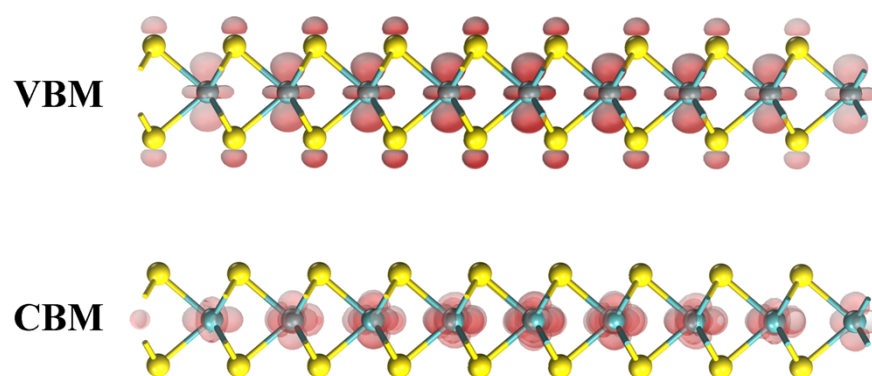


Figure S2. The partial charge density for the CBM and VBM of MoS₂ML.

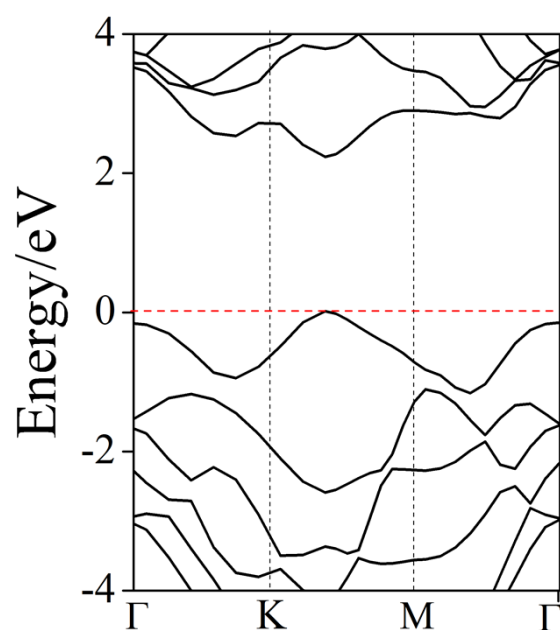


Figure S3. Band structure of MoS₂ML computed by using HSE06 functional.

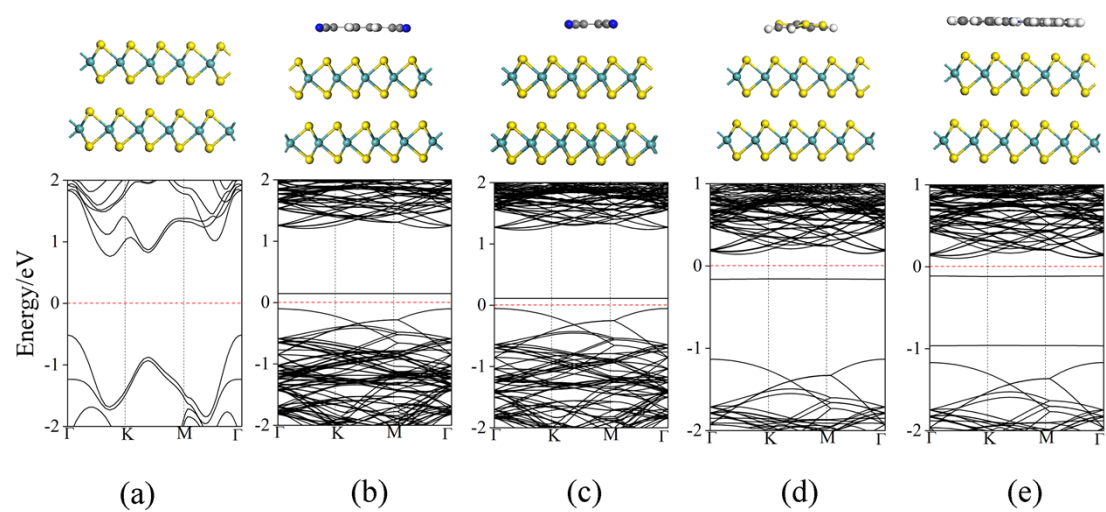


Figure S4. Geometric structures (upper) and band structures (bottom) of free-standing MoS_2BL (a) as well as those functionalized with TCNQ (b), TCNE (c), TTF (d), and BV (e).