Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

N-type and p-type molecular doping on monolayer MoS_2

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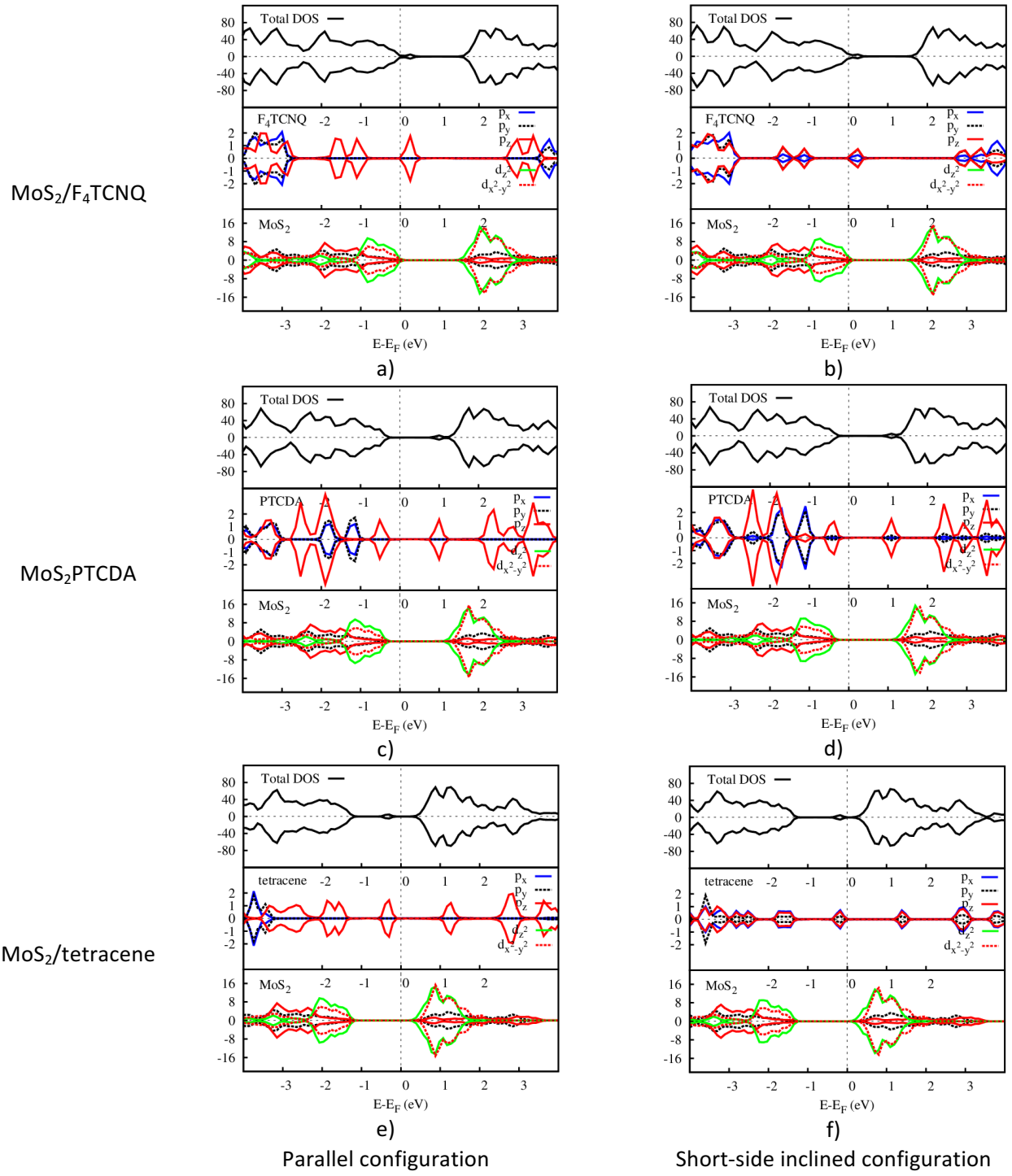

Fig. S1 Electronic density of states of MoS_2/F_4TCNQ, MoS_2/PTCDA, and MoS_2/tetracene for the most favorable configuration (the short-side inclined) and the parallel configuration. The DOS is almost the same for the parallel and short-side inclined configurations.

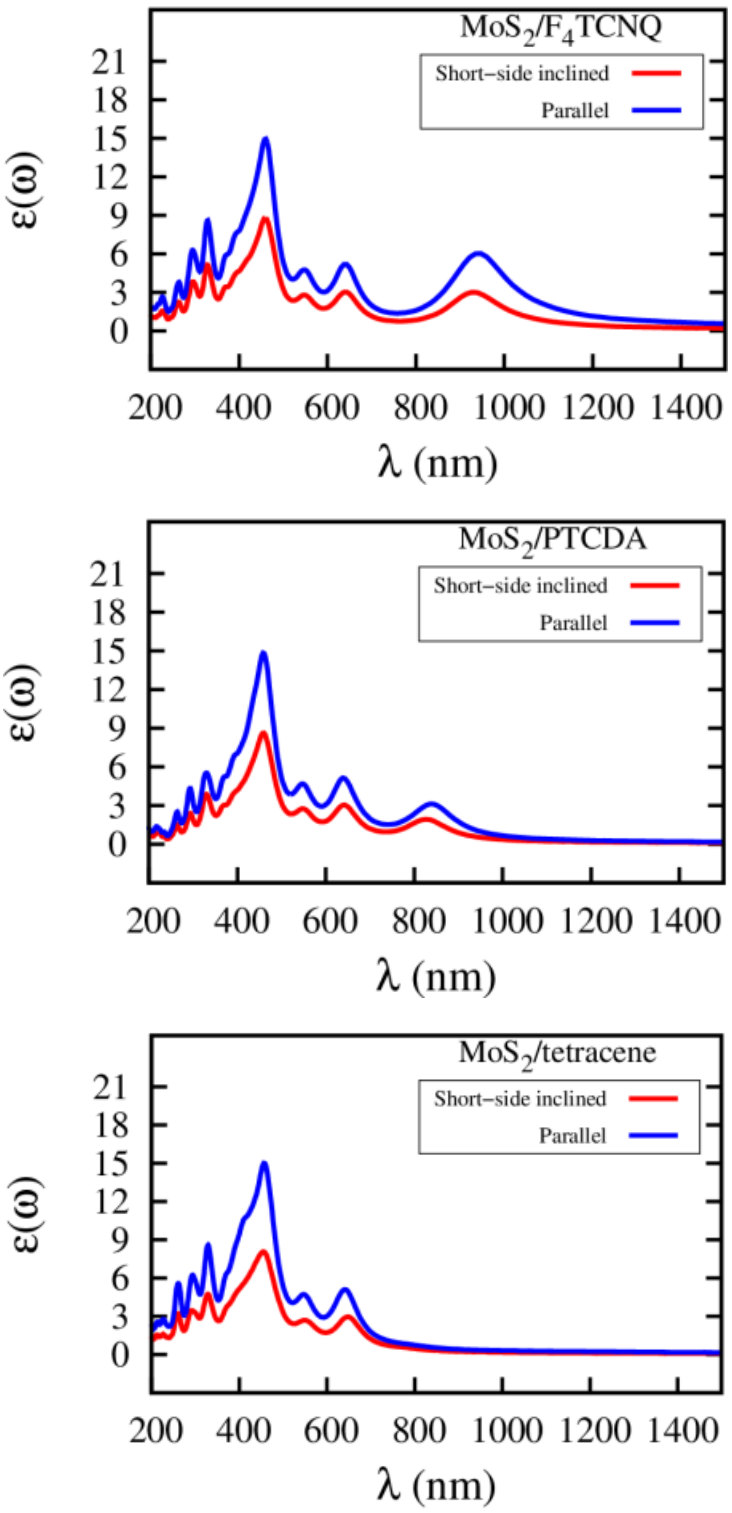

Fig. S2 Imaginary part of dielectric function ε(ω) versus wavelength λ for MoS_2/F_4TCNQ, MoS_2/PTCDA, and MoS_2/tetracene at zero pressure for different configurations and vacuum spaces.

Table S1 The adsorpion energy (eV) of the molecules on the monolayer MoS_2.

Unit cell	MoS_2/F_4TCNQ	MoS_2/PTCDA	MoS_2/tetracene
5x5	-0.009	0.019	0.039
6x6	-0.028	-0.010	0.008

Table S2 The adsorpion energy (eV) of the molecules on the monolayer MoS_2 with and without the inclusion of van der Waals dispersion correction.

Functional	F_4TCNQ	PTCDA	tetracene
Without vdW (PBE)	-0.009	0.019	0.039
vdW-DF (revPBE)*	-1.109	-1.664	-1.205

* M. Dion, H. Rydberg, E. Schröder, D. C. Langreth, B. I. Lundqvist, Phys. Rev. Lett. 92, 246401 (2004)

Table S3 The bandgap E_g (eV) of MoS_2/F_4TCNQ, MoS_2/PTCDA, and MoS_2/tetracene systems with and without the van der Waals dispersion correction.

Functional	Isolated MoS_2	F_4TCNQ	PTCDA	tetracene
Without vdW (PBE)	1.68	0.36	1.43	0.72
vdW-DF (revPBE)*	1.70	0.40	1.45	0.60

The adsorption energy for a larger unit cell size and with van der Waals correction is more negative than the 5 x 5 unit cell without vdW correction. However, the DOS remains the same for all of them (see Fig. S3). The inclusion of vdW correction slightly modifies the bandgap.

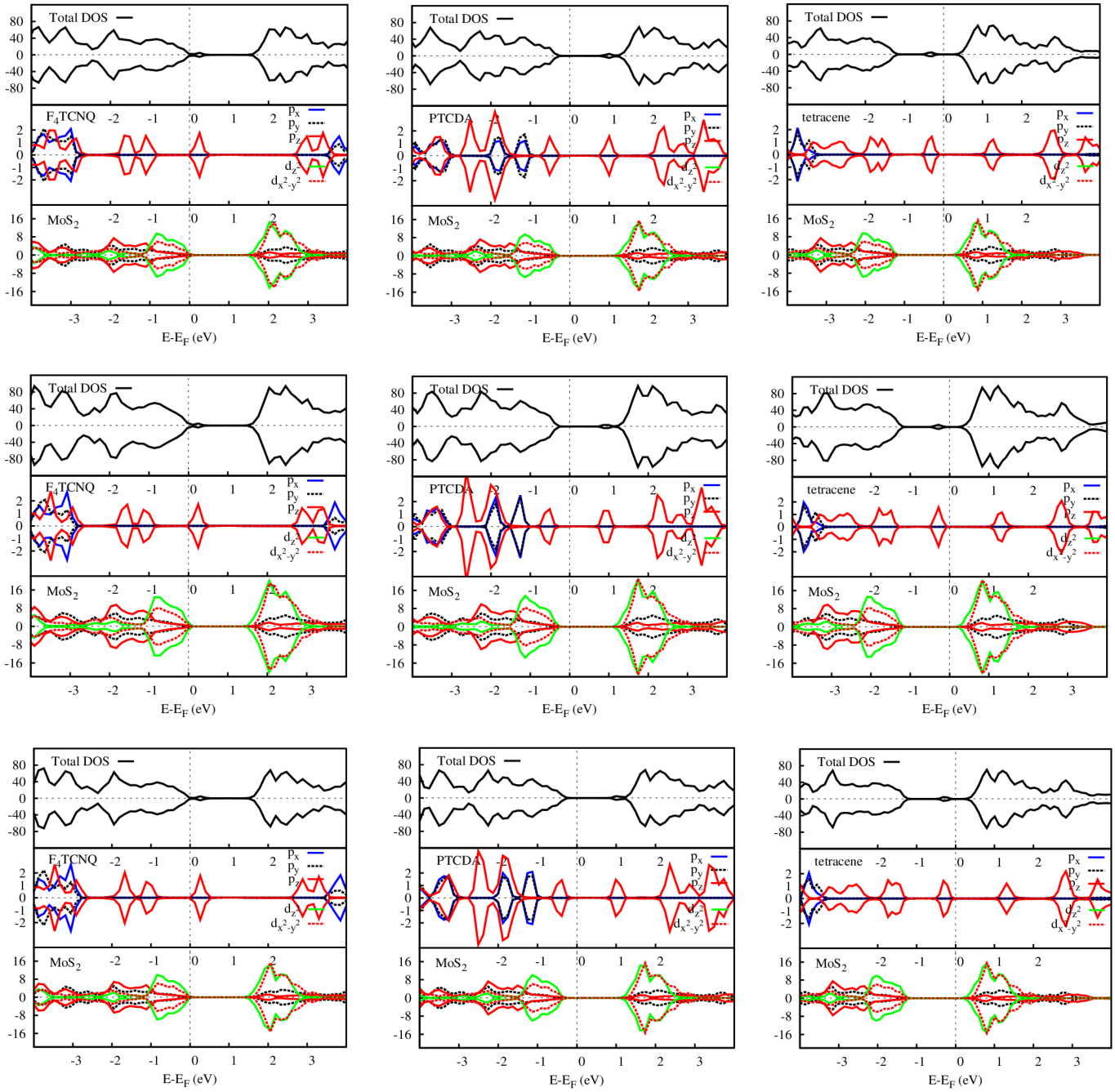

Fig. S3 From left to right, electronic density of states of MoS_2/F_4TCNQ, MoS_2PTCDA, and MoS_2/tetracene with the parallel adsorption configuration. The first to third rows are those for the 5 × 5 unit cell, the 6 × 6 unit cell of the monolayer MoS_2, and taking into account the van der Waals correction, respectively.