Supplementary Information

N-type and p-type molecular doping on monolayer MoS₂

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**Fig. S1** Electronic density of states of MoS$_2$/F$_4$TCNQ, 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 $\varepsilon(\omega)$ versus wavelength $\lambda$ for MoS$_2$/F$_4$TCNQ, MoS$_2$/PTCDA, and MoS$_2$/tetracene at zero pressure for different configurations and vacuum spaces.
Table S1 The adsorption energy (eV) of the molecules on the monolayer MoS$_2$.

| Unit cell | MoS$_2$/F$_4$TCNQ | MoS$_2$/PTCDA | MoS$_2$/tetracene |
|-----------|------------------|---------------|-------------------|
| 5x5       | -0.009           | 0.019         | 0.039             |
| 6x6       | -0.028           | -0.010        | 0.008             |

Table S2 The adsorption energy (eV) of the molecules on the monolayer MoS$_2$ with and without the inclusion of van der Waals dispersion correction.

| Functional | F$_4$TCNQ | 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$_4$TCNQ, MoS$_2$/PTCDA, and MoS$_2$/tetracene systems with and without the van der Waals dispersion correction.

| Functional | Isolated MoS$_2$ | F$_4$TCNQ | 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$_4$TCNQ, MoS$_2$PTCDA, 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.