Electronic Supplementary Material (ESI) for CrystEngComm.

Electronic Supplementary Information

Charge injection phenomena at the contact interface between (5,10,15,20-tetramethylporphyrinato)cobalt(II) and 2,5-difluoro-7,7,8,8-tetracyanoquinodimethane single crystals

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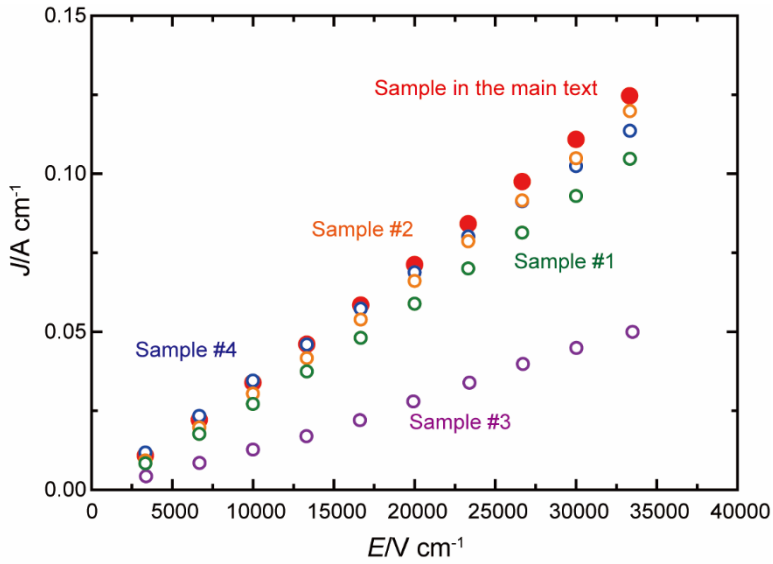

Figure S1. Sample dependence of the current-voltage characteristics of the CoTMP/F_2TCNQ interface. The current-voltage characteristics of five interfaces, including the one adopted in the main text (red), are shown.

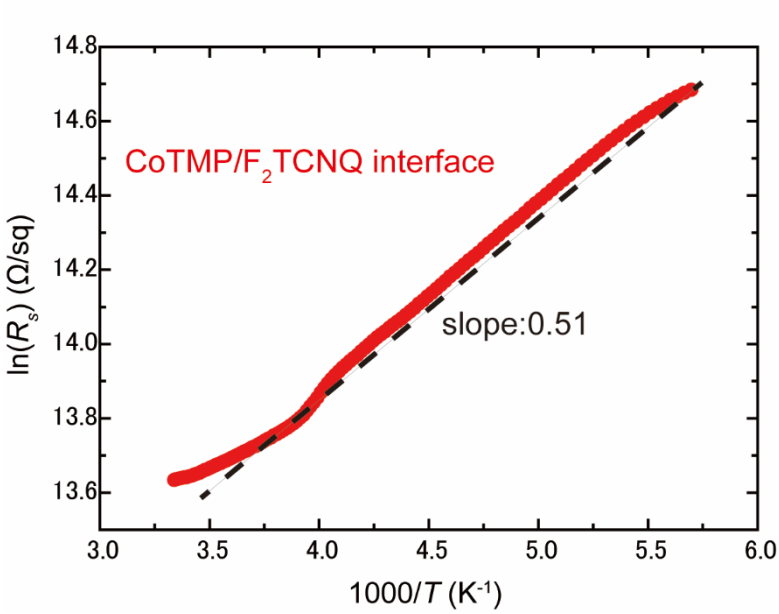

Figure S2. The temperature dependence of the sheet resistance at the CoTMP/F_2TCNQ interface (red dot) is shown in an Arrhenius plot. It shows an almost linear relationship to the inverse of the temperature, which indicates that this interface is semiconducting behavior. The slope of the approximate line (black dashed line) is 0.51. This slope and the equation (Rs = A*exp(-Ea/$k_B T$)) provide the activation energy (Ea) of the semiconducting interface, where Rs, A, k_B, and T are sheet resistance, frequency factor, Boltzman constant, and temperature. As a result, the Ea was found to be 0.04 eV.

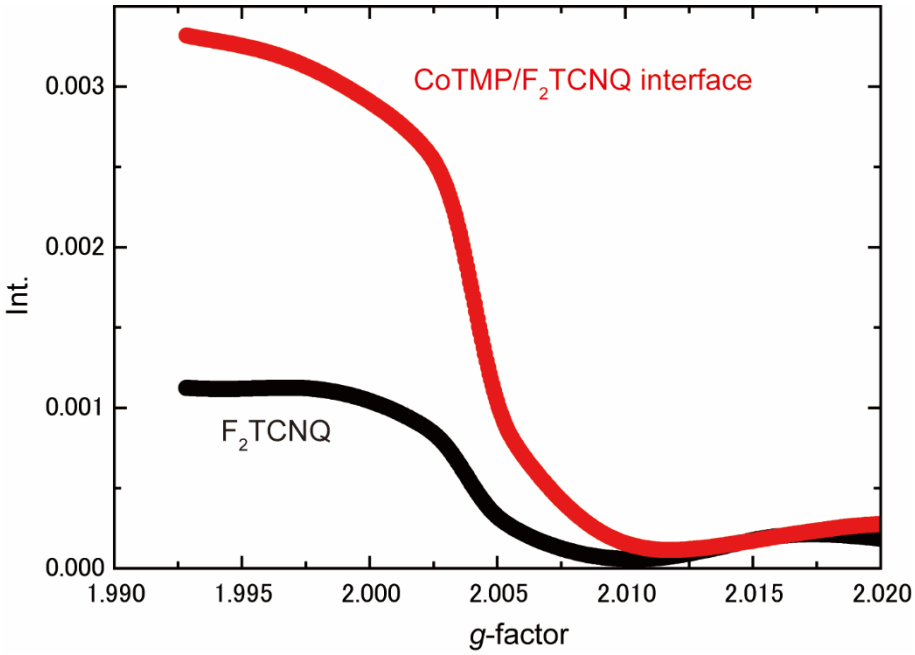

Figure S3. ESR intensity plot of the spectra in Figure 4 in the main text, integrated twice. The number of charged molecules (N_{charge}= 0.0054 × 10^{13}) can be determined from the following equation; N_{charge} = ($I_{interface}$ - I_{F2TCNQ})/ I_{ion}, where $I_{interface}$ (= 0.0033) and I_{F2TCNQ} (= 0.0011) are the two times integrated ESR spectrum of the contact interface and F_2TCNQ, respectively. And I_{ion} (= 0.41 × 10^{-13}) is the integrated intensity of one radical, which is determined with using Cobalt(II) Phthalocyanine. The number of molecules in the single interfacial molecular ($N_{interface}$ = 0.048 × 10^{13}) can be calculated from the contact area (S = 0.3 mm × 0.5 mm) and the lattice constant of the surface (CoTMP:11.48 Å× 5.52 Å, F_2TCNQ:10.21 Å× 6.03 Å). As a result, the number of molecules ionized at the interface is 11%.

Table S1.1 The reflection indices of F_2TCNQ

h	*k*	*l*	2θ (degree)
0	0	1	10.469
1	1	0	17.277
2	0	-1	18.146
1	1	-1	18.826
0	0	2	20.986
1	1	1	21.573
2	0	1	23.474
2	0	-2	23.521
1	1	-2	25.188
1	1	2	29.296
0	2	0	29.601

Table S1.2 The reflection indices of CoTMP

h	*k*	*l*	2θ (degree)
1	0	0	8.022
0	0	2	12.8
1	0	-2	13.239
0	1	1	17.5
1	1	-1	18.585
0	1	2	20.806
1	1	-2	21.064
3	0	0	24.292
1	0	-4	24.895
0	1	3	25.323
3	1	-1	28.675
1	0	4	29.065