

Fig. S1. The optimized geometries for compounds 1-3 and new conformers not showing in the crystal named as 1'-3' (at B3LYP/6-31G\* level).

Table S1.	The electronic	energy	including	the	zero-point	energy	corrections	and	the	relative	energy	between
staggered	and parallel isor	ners for	systems 1-	3.								

	Net	utral State	Cationic State			
Compounds	Energy (hartree)	Relative Energy(meV)	Energy (hartree)	Relative Energy(meV)		
1 (parallel form)	-2901.1037	0.00	-2900.9000	0.00		
1' (staggered form)	-2901.1040	-8.03	-2900.9017	-44.65		
<b>2</b> (parallel form)	-2979.6850	0.00	-2979.4842	0.00		
2' (staggered form)	-2979.6854	-10.39	-2979.4861	-51.73		
3' (parallel form)	-3820.3148	0.00	-3820.1053	0.00		
<b>3</b> (staggered form)	-3820.3152	-10.72	-3820.1071	-48.41		



Fig. S2. Contributions of individual vibrational mode to the relaxation energies for both neutral and cationic states. (a) neutral 1, (b) cationic 1, (c) neutral 2, (d) cationic 2, (e) neutral 3, (f) cationic 3.



Fig. S3. The relative position of the dimer exhibiting the largest transfer integral, i.e. P3 of system 1, P3 of system 2, and P2 of system 3. (a) The definition of the long molecular axis and short molecular axis; (b) Side view along the long axis and (c) the corresponding overlaps of HOMOs; (d) Side view along the short axis and (e) the corresponding overlaps of HOMOs; (f) Top view of the dimer.