

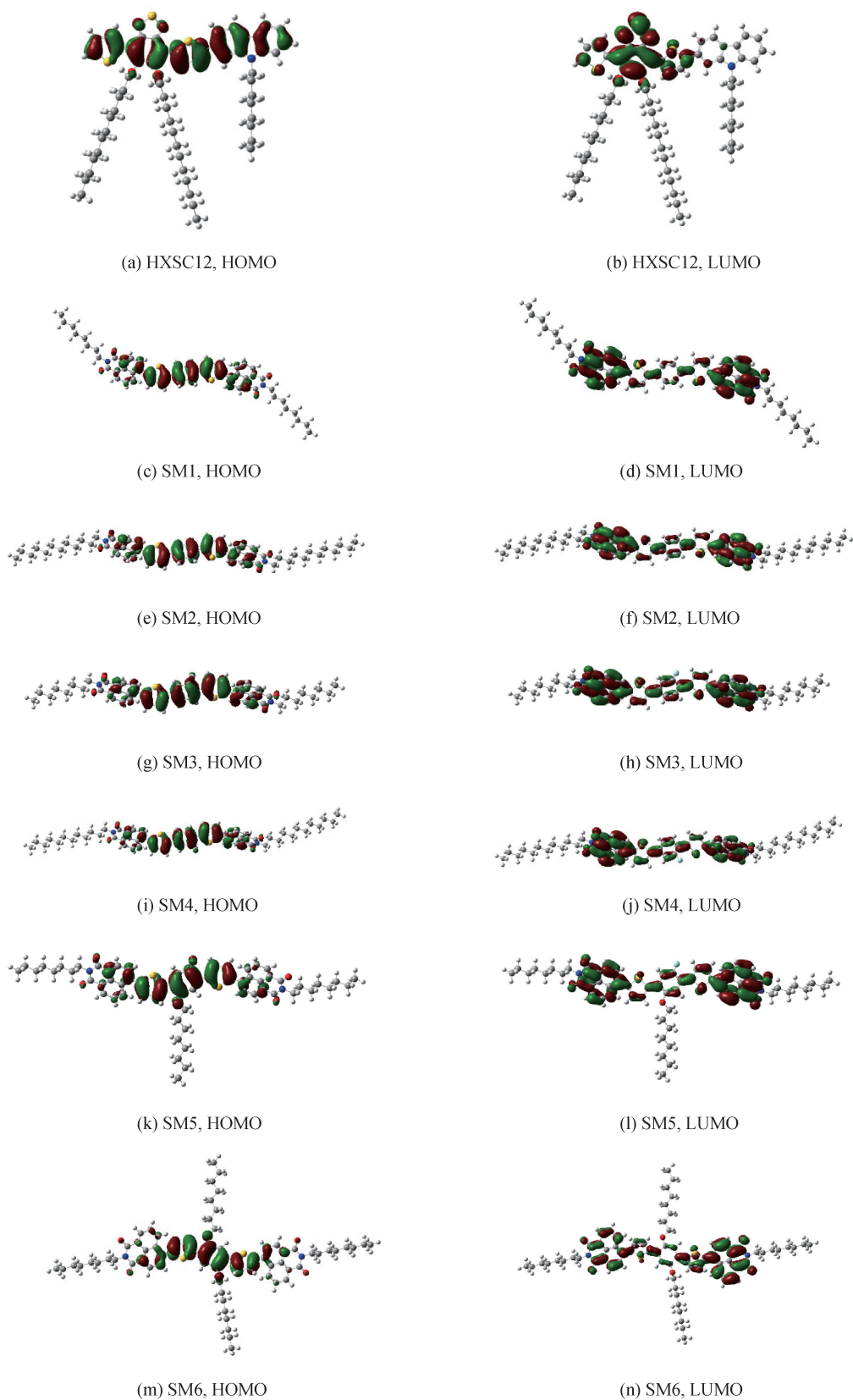


图 S1 HXSC12 和 SM1~SM6 的分子轨道

Fig. S1 The molecule orbitals of HXSC12 and SM1-SM6

表 S1 ED1 和 ED2 过程的重组能

Tab, S1 The results of reorganization energy for ED1 and ED2 eV

体系	ED1			ED2		
	λ_1	λ_2	λ	λ_1	λ_2	λ
HXSC12-SM1	0.130	0.212	0.342	0.285	0.117	0.402
HXSC12-SM2	0.130	0.173	0.303	0.285	0.111	0.396
HXSC12-SM3	0.130	0.192	0.322	0.285	0.076	0.361
HXSC12-SM4	0.130	0.223	0.353	0.285	0.206	0.491
HXSC12-SM5	0.130	0.196	0.326	0.285	0.079	0.364
HXSC12-SM6	0.130	0.168	0.298	0.285	0.110	0.395

表 S2 ED1 和 ED2 过程的驱动力

Tab, S2 The driving force for ED1 and ED2 eV

体系	$E(D^+/D^-)$	$E(A/A^-)$	E_{cb}	ED1		ED2	
				ΔE_{00}	ΔG	ΔE_{00}	ΔG
HXSC12-SM1	5.587	3.010	-0.189	2.451	-0.063	2.522	-0.134
HXSC12-SM2	5.587	3.002	-0.194	2.451	-0.060	2.538	-0.147
HXSC12-SM3	5.587	3.057	-0.215	2.451	-0.136	2.571	-0.256
HXSC12-SM4	5.587	3.223	-0.191	2.451	-0.278	2.529	-0.356
HXSC12-SM5	5.587	3.043	-0.189	2.451	-0.096	2.506	-0.151
HXSC12-SM6	5.587	2.915	-0.232	2.451	-0.011	2.554	-0.114

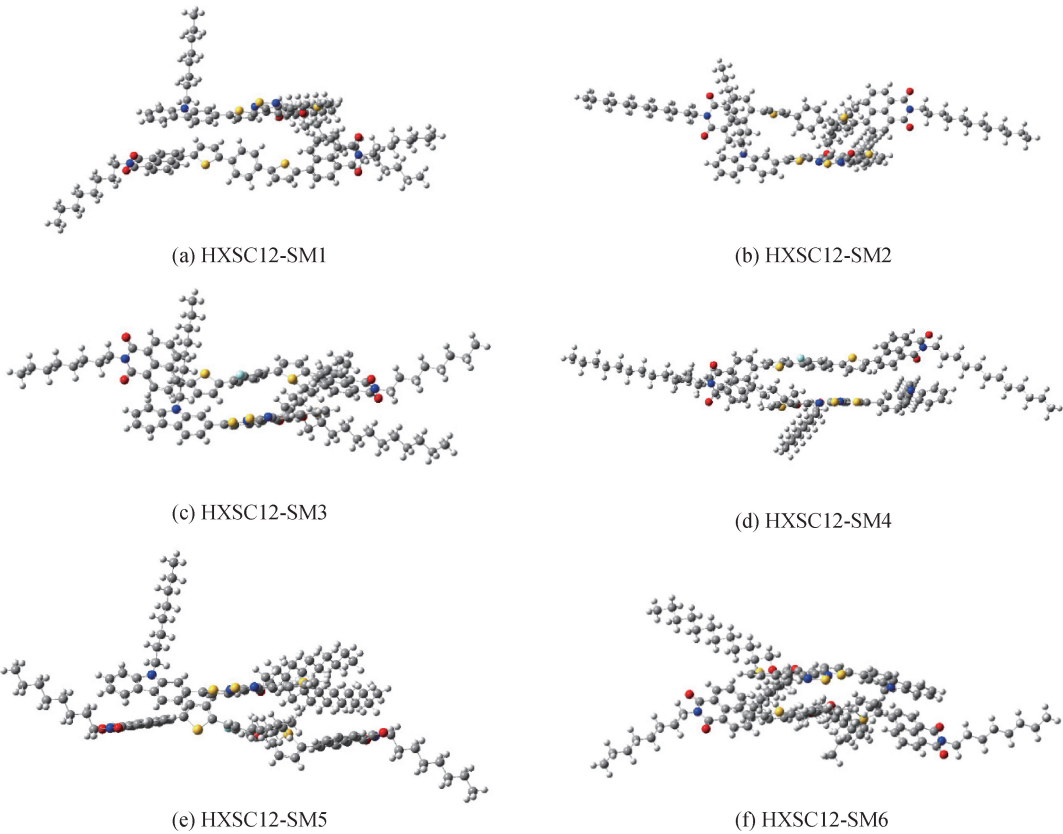


图 S2 6 个体系的相对构型
Fig, S2 The relative geometries of 6 systems