DFT Result

Table S3. The chemical descriptor of compound (All values in eV)

Compound	E_{HOMO}	E_{LUMO}	ΔE_{gap}	I	A	χ	η	ω
C1	-6.5318	-2.5652	3.9666	6.5318	2.5652	4.5485	1.9833	20.5163
C2	-6.1046	-2.4003	3.7043	6.1046	2.4003	4.2525	1.8521	16.7466
C3	-6.2140	-2.5679	3.6461	6.2140	2.5679	4.3910	1.8230	17.5745
C4	-6.3952	-2.5489	3.8463	6.3952	2.5489	4.4721	1.9232	19.2310
C5	-5.9525	-2.4270	3.5255	5.9525	2.4270	4.1897	1.7628	15.4716
C6	-6.7465	-2.7337	4.0129	6.7465	2.7337	4.7401	2.0064	22.5407
C7	-6.6967	-2.7590	3.9378	6.6967	2.7590	4.7278	1.9689	22.0047
C8	-6.1615	-2.6379	3.5236	6.1615	2.6379	4.3997	1.7618	17.0517
C9	-6.0586	-2.6477	3.4109	6.0586	2.6477	4.3531	1.7055	16.1593