Supplementary Information: Investigation of Structural and Optoelectronic Properties of Organic Semiconductor Film based on 8-hydroxiquinoline Zinc

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Table SM1. Distances calculated for the hydrogen bridges formed between ZnQ$_2$ and TCNQ, and HOMO-LUMO gap (E$_g$).

	B3PW91/6-31G**	PBE/TZ2P
d$_{N-H}$ (Å)	2.680	2.473
d$_{O-H}$ (Å)	2.337	2.440
E$_g$ (eV)	1.353	0.017

Table SM2. Molecular electronic transitions calculated for ZnQ$_2$-TCNQ using TDDFT-PBE/TZ2P method, and the parameters characterizing them: energy electronic transition (E$_T$), oscillator strength (f), transition from occupied molecular orbital to unoccupied molecular orbital, and weight of the transition.

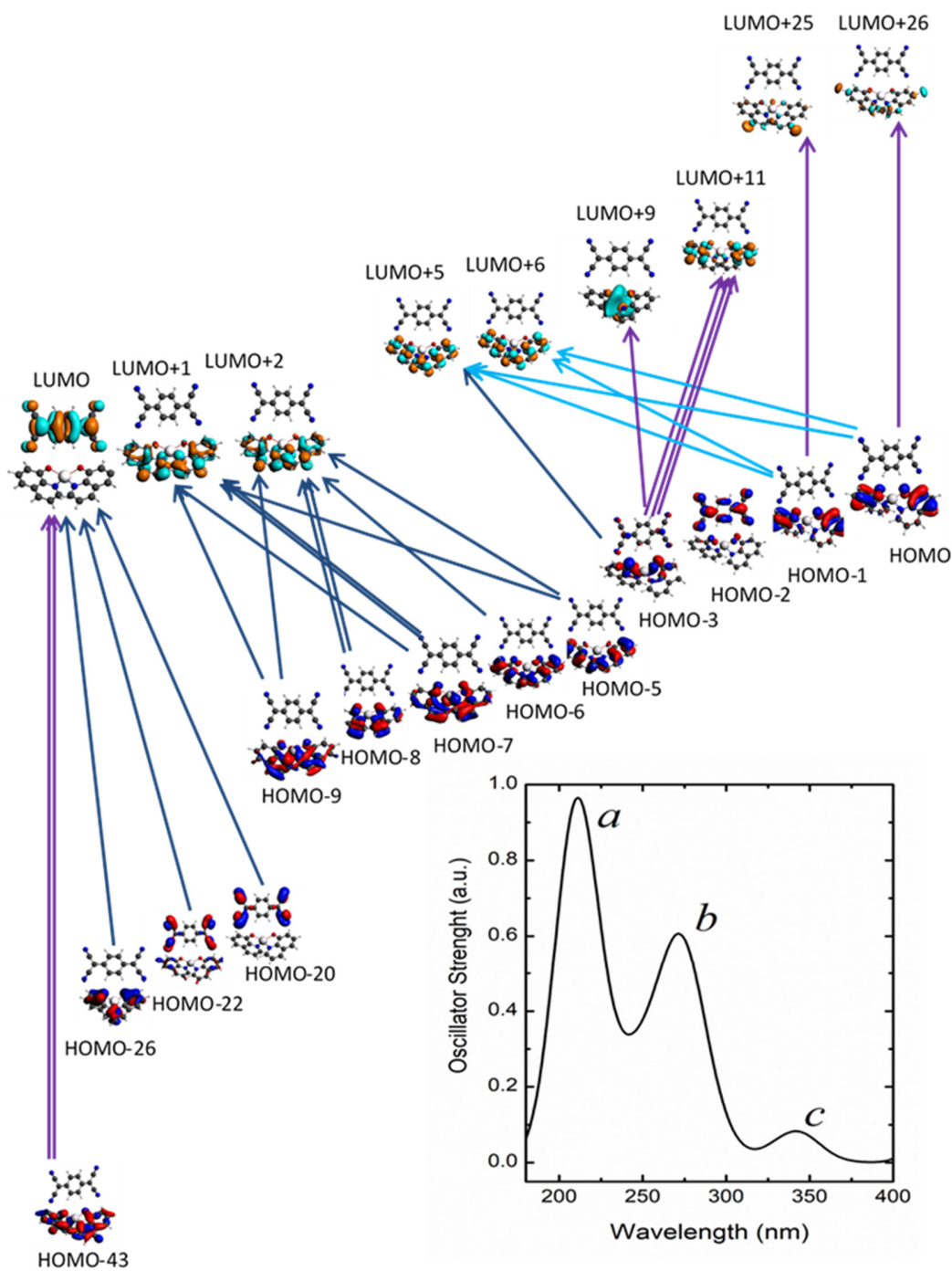| Band	E$_T$ (nm)	E$_T$ (eV)	f (u.a.)	Molecular Electronic Transition			Weight (%)
c	339.96	3.647	0.040	HOMO	→	LUMO+6	37.6
				HOMO-1	→	LUMO+5	35.5
	339.68	3.650	0.019	HOMO-1	→	LUMO+6	39.4
				HOMO	→	LUMO+5	30.7
b	289.01	4.290	0.061	HOMO-20	→	LUMO	35.1
				HOMO-22	→	LUMO	27.4
				HOMO-26	→	LUMO	27.8
	273.14	4.539	0.019	HOMO -7	→	LUMO+1	46.91
				HOMO -8	→	LUMO+2	36.57
	271.24	4.571	0.212	HOMO-5	→	LUMO+1	22.5
				HOMO-6	→	LUMO+2	19.5
				HOMO-8	→	LUMO+2	13.5
	270.41	4.585	0.185	HOMO-5	→	LUMO+2	27.9
				HOMO-6	→	LUMO+1	23.0
	266.34	4.655	0.031	HOMO -9	→	LUMO+2	54.47
				HOMO -7	→	LUMO+2	25.02
	265.43	4.671	0.064	HOMO-9	→	LUMO+1	52.4
				HOMO -7	→	LUMO+1	21.8
	261.95	4.733	0.028	HOMO -3	→	LUMO+5	66.83
a	214.10	5.791	0.185	HOMO -3	→	LUMO+9	61.1
	212.41	5.837	0.126	HOMO -1	→	LUMO+25	76.0
	209.72	5.912	0.134	HOMO	→	LUMO+26	33.7
				HOMO -3	→	LUMO+11	13.5
	206.71	5.998	0.107	HOMO -43	→	LUMO	44.9
				HOMO -3	→	LUMO+11	12.9
	206.61	6.001	0.126	HOMO -43	→	LUMO	50.2
				HOMO -3	→	LUMO+11	20.9

Figure SM1. Schematization of the main molecular electronic transitions fashioning the bands in the absorption spectrum. Color code: purple arrows represent the transitions in band *a*; blue arrows correspond to transitions in band *b;* and light blue arrows represent the transitions in band *c*.

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Table SM3. Electronic transitions singlet-singlet with energy comparable to the experimental optical gap $E_{opt} = 2.4$ eV, and with a higher probability of occurrence.

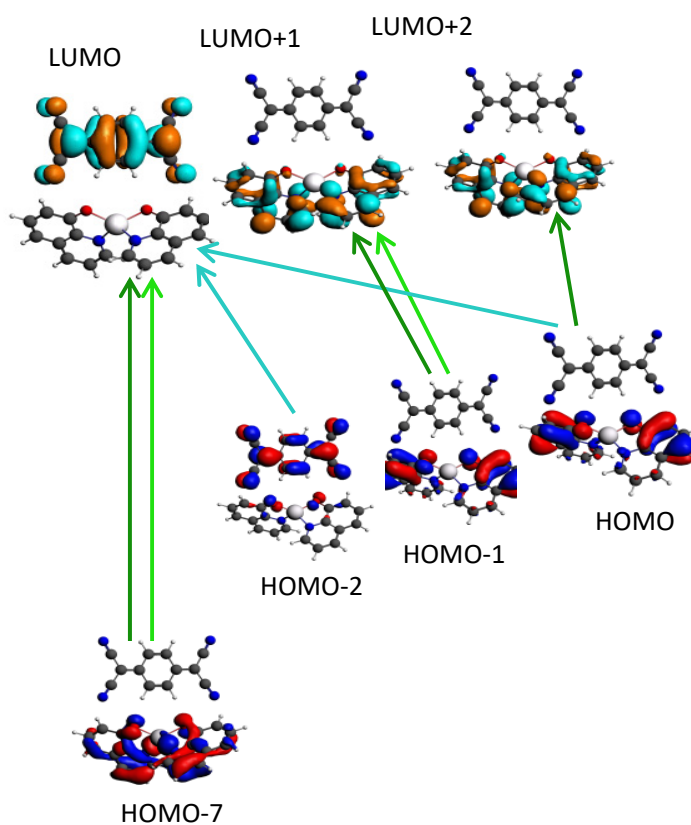| E_T (eV)	f (u.a.)	Molecular Electronic Transition			Weight (%)
2.393	0.016	HOMO -7	→	LUMO	63.3
		HOMO -1	→	LUMO+1	18.1
2.434	0.028	HOMO -7	→	LUMO	33.5
		HOMO -1	→	LUMO+1	28.4
		HOMO	→	LUMO+2	26.3
2.636	0.410	HOMO -2	→	LUMO	56.0
		HOMO	→	LUMO	26.3

Figure SM2. Schematization of the electronic transitions singlet-singlet with energy comparable to the experimental optical gap $E_{opt} = 2.4$ eV, and with a higher probability of occurrence (see table SM3).