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新型四硫富瓦烯-三苯胺类光敏染料理论研究

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Theoretical Investigation of Novel Tetrathiafulvalene-Triphenylamine Sensitizers

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Table S1 Electronic transition configurations, computed excitation energies and oscillator strengths (*f*) for the optical transitions with *f* > 0.01 of the absorption bands in visible and near UV region for YD1-3 before and after binding to $(TiO_2)_9$ clusters in vacuum. (H = HOMO, L = LUMO, L + 1 = LUMO + 1, etc.)

Dye	λ/nm	*E*/eV	*f*	Composition	
YD1	363.8	3.41	1.0097	H → L(+93%)	
	261.4	4.74	0.1575	H → L + 2(+44%),	H → L + 1(+32%)
				H – 4 → L(+7%)	
	252.3	4.92	0.1143	H – 1 → L(+74%),	H → L + 3(+5%)
YD2	377.2	3.29	1.4272	H – 1 → L(+65%),	H → L(+17%)
				H – 2 → L(5%)	
	319.3	3.88	0.9357	H → L + 1(+50%),	H – 1 → L + 1(+14%)
				H – 1 → L(+10%)	
	294.7	4.21	0.1185	H → L(+59%),	H – 1 → L + 1(+25%)
	257.0	4.82	0.1109	H – 6 → L(+19%),	H – 3 → L + 1(+16%)
				H – 5 → L(11%),	H – 2 → L(7%)
				H – 3 → L(6%),	H – 2 → L + 1(6%)
	244.6	5.07	0.4106	H → L + 8(+15%),	H → L + 9(+9%)
				H – 2 → L + 1(+8%),	H – 3 → L + 2(8%)
				H → L + 1(7%),	H – 2 → L + 2(7%)
				H – 6 → L(6%)	
YD3	378.1	3.28	1.3770	H – 2 → L(+57%),	H → L(+21%)
				H – 4 → L(6%)	
	345.7	3.59	2.2794	H → L + 1(+39%) ,	H – 2 → L + 1(+30%)
				H – 1 → L + 2(7%)	
	290.9	4.26	0.1316	H → L(+59%),	H → L + 2(+6%)
				H – 2 → L(6%)	
	265.7	4.67	0.1253	H – 4 → L + 1(+15%),	H – 2 → L + 9(11%)
				H – 18 → L(7%),	H – 3 → L(6%)
				H – 14 → L(+5%)	
YD1-$(TiO_2)_9$	391.0	3.17	1.5535	H → L + 10(+31%),	H → L + 8(28%)
				H → L + 6(+15%),	H → L + 5(+8%)
YD2-$(TiO_2)_9$	406.2	3.05	1.7861	H – 1 → L + 8(+18%),	H – 1 → L + 6(+15%)
				H – 1 → L + 5(13%),	H – 1 → L + 9(13%)
	348.3	3.56	0.1314	H → L + 5(+36%),	H → L + 6(21%)
				H → L + 8(13%),	H → L + 9(+5%)
	323.6	3.83	0.6300	H → L + 24(+31%),	H → L + 8(+30%)
				H – 1 → L + 24(+9%),	H → L + 23(7%)
	316.3	3.92	0.1362	H → L + 9(+75%),	H → L + 24(7%)
				H → L + 8(+5%)	
YD3-$(TiO_2)_9$	406.3	3.05	1.8525	H – 2 → L + 5(+21%),	H – 2 → L + 8(12%)
				H – 2 → L + 6(+11%),	H → L + 5(+8%)
				H – 2 → L + 9(8%)	
	355.4	3.49	1.0475	H – 1 → L + 5(+24%),	H → L + 21(+15%)
				H – 1 → L + 6(+9%),	H – 2 → L + 21(+8%)
				H – 1 → L + 8(8%)	
	344.1	3.60	0.1062	H → L + 5(+51%),	H → L + 6(+12%)
				H → L + 8(5%)	
	337.7	3.67	0.9205	H – 1 → L + 5(+39%),	H → L + 21(17%)
				H – 2 → L + 21(15%),	H – 1 → L + 6(+7%)

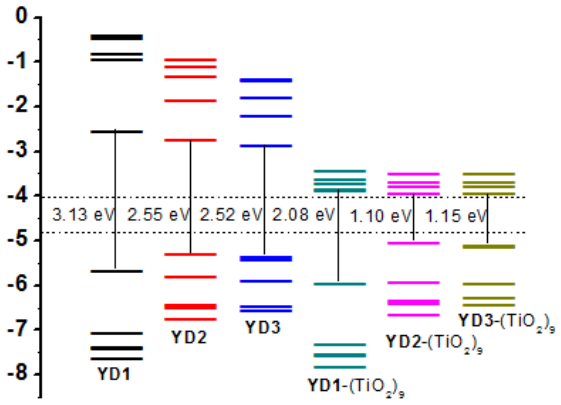

Fig.S1 Molecular orbital energy diagram of YD1-3 before and after binding to $(TiO_2)_9$ clusters by B3LYP hybrid functional alone with 6-31G*for C, H, O, N, S atoms, effective core potential (ECP) LANL2DZ and its accompanying basis set for Ti atom

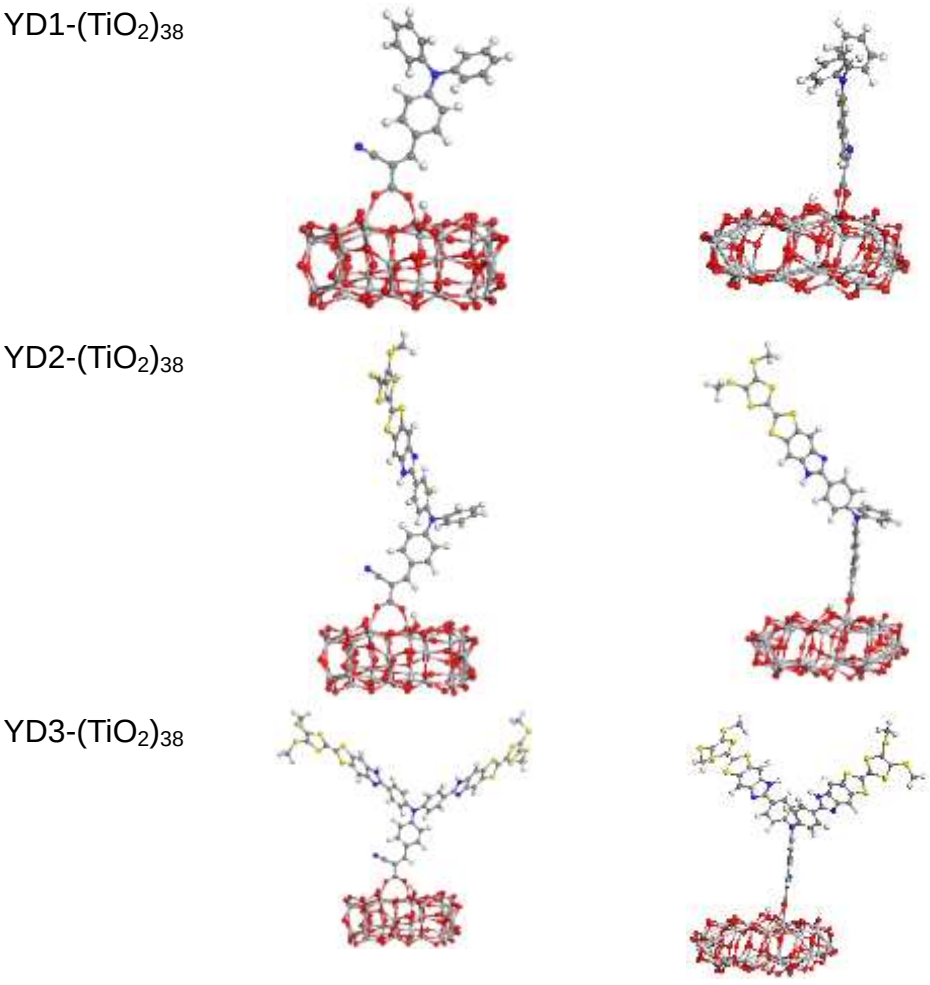

Fig.S2 Optimized structures of YD1, YD2 and YD3 adsorbed on $(TiO_2)_{38}$ (101) surface by DMol^3 calculation