

Supplementary Information

**Theoretical Studies on the Quinoidal Thiophene Based Dyes for Dye Sensitized Solar Cell
and NLO applications**

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Table S1 The absorption wavelength (in nm and eV) associated with HOMO → LUMO transition in QT1 dye molecule calculated at (a) different methods (b) in basis sets in acetonitrile medium.

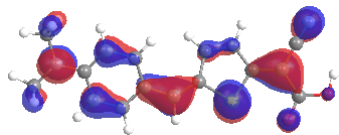
(a)

Method	Transition	λ_{abs}		f
		nm	eV	
B3LYP/6-311G(d,p)	H→L	529	2.34	1.375
PBE0/6-311G(d,p)	H→L	520	2.38	1.420
M06-2X/6-311G(d,p)	H→L	505	2.46	1.478
M06-HF/6-311G(d,p)	H→L	490	2.53	1.525
CAM-B3LYP/6-311G(d,p)	H→L	498	2.49	1.489
LC-BLYP/6-311G(d,p)	H→L	472	2.63	1.576
BHandHLYP/6-311G(d,p)	H→L	483	2.57	1.533

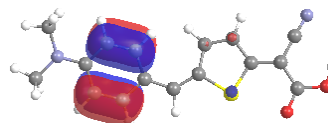
(b)

Basis set	Transition	λ_{abs}		f
		nm	eV	
6-311+G(d,p)	H→L	537	2.31	1.389
6-311++G(d,p)	H→L	537	2.31	1.388
6-311G(2d, p)	H→L	530	2.34	1.369
6-311+G(2d,p)	H→L	538	2.30	1.383
6-311G(2d,2p)	H→L	531	2.34	1.369
6-311+G(2d,2p)	H→L	539	2.30	1.382

Experimental absorption wavelength of QT1 molecule is **548 nm** in acetonitrile medium.

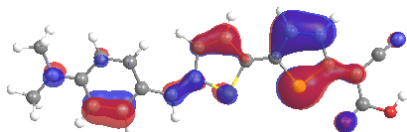


HOMO-1

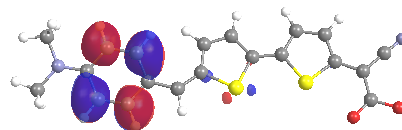


HOMO-2

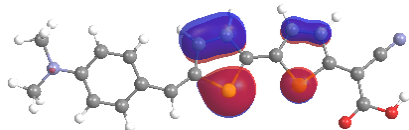
QT1



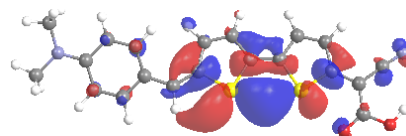
HOMO-3



LUMO+2

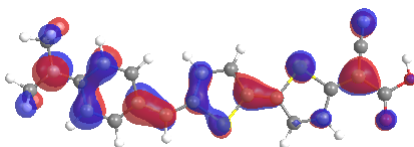


HOMO-5

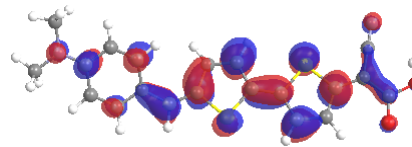


LUMO+3

QT2A

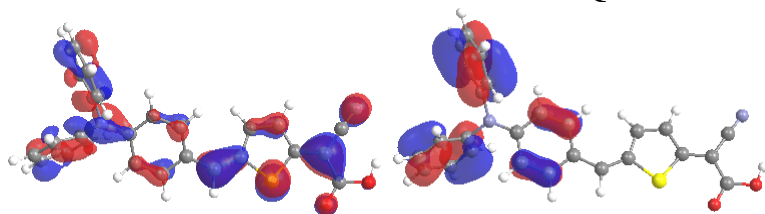


HOMO-1



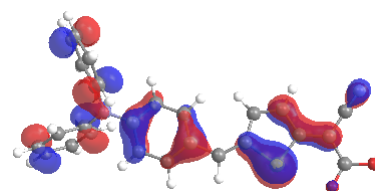
LUMO+1

QT2B

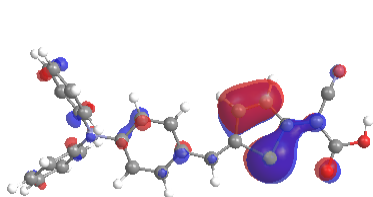


HOMO-1

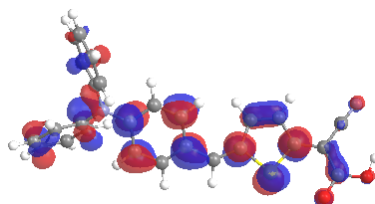
HOMO-3



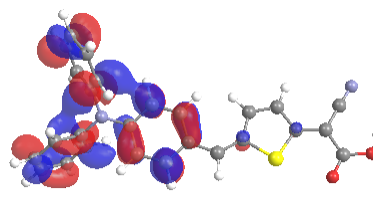
HOMO-4



HOMO-7

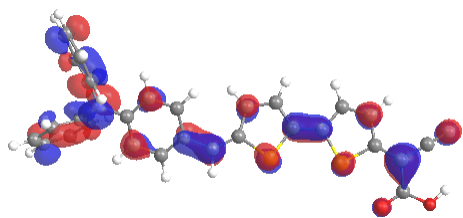


LUMO+1

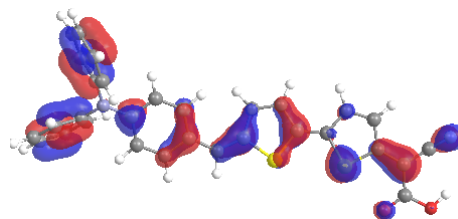


LUMO+2

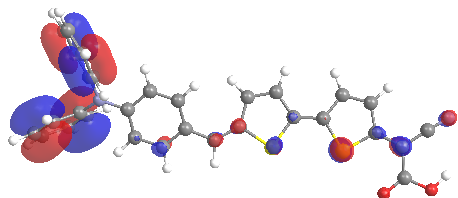
QT3



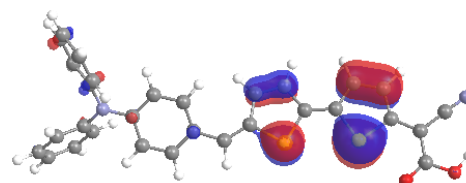
HOMO-1



HOMO-2

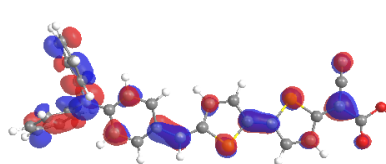


HOMO-3

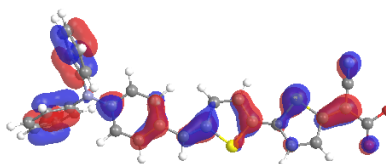


HOMO-5

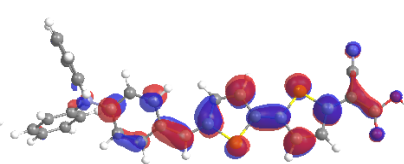
QT4A



HOMO-1

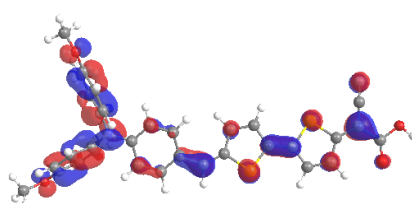


HOMO-2

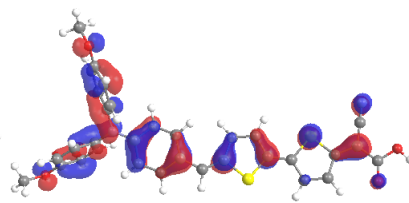


LUMO+1

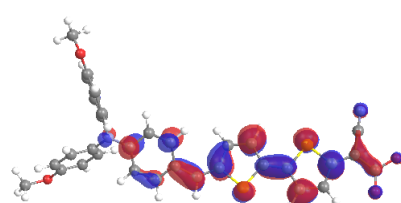
QT4B



HOMO-1

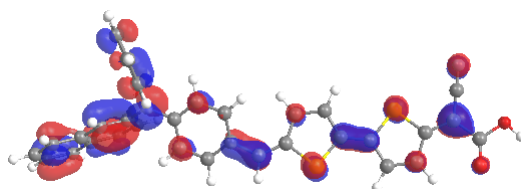


HOMO-3

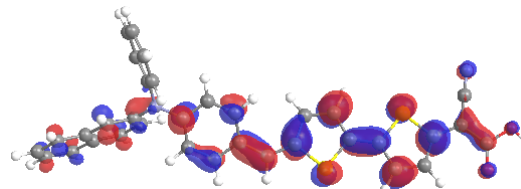


LUMO+1

QT5



HOMO-1



LUMO+1

QT6

