

# A promising small-sized near-infrared absorbing zwitterionic dyes for DSSC and NLO applications: DFT and TD-DFT approach

Suryapratap J. Sharma, and Nagaiyan Sekar\*

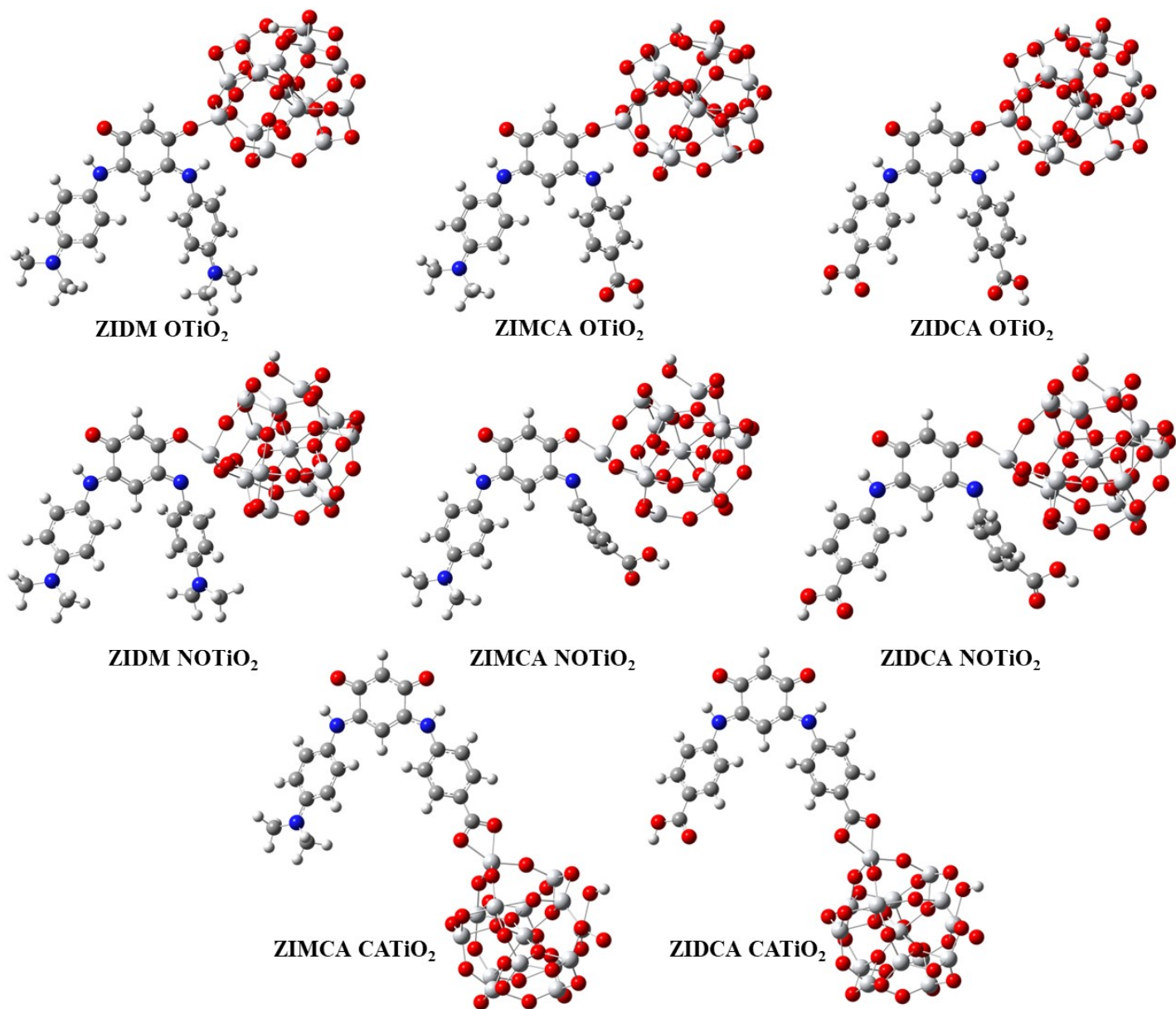
Dyestuff Technology Department (Currently named as Department of Speciality Chemicals Technology), Institute of Chemical Technology, N. P. Marg, Matunga, Mumbai, 400019, Maharashtra, India

E-mail: [nethi.sekar@gmail.com](mailto:nethi.sekar@gmail.com), [n.sekar@ictmumbai.edu.in](mailto:n.sekar@ictmumbai.edu.in) (N. Sekar)

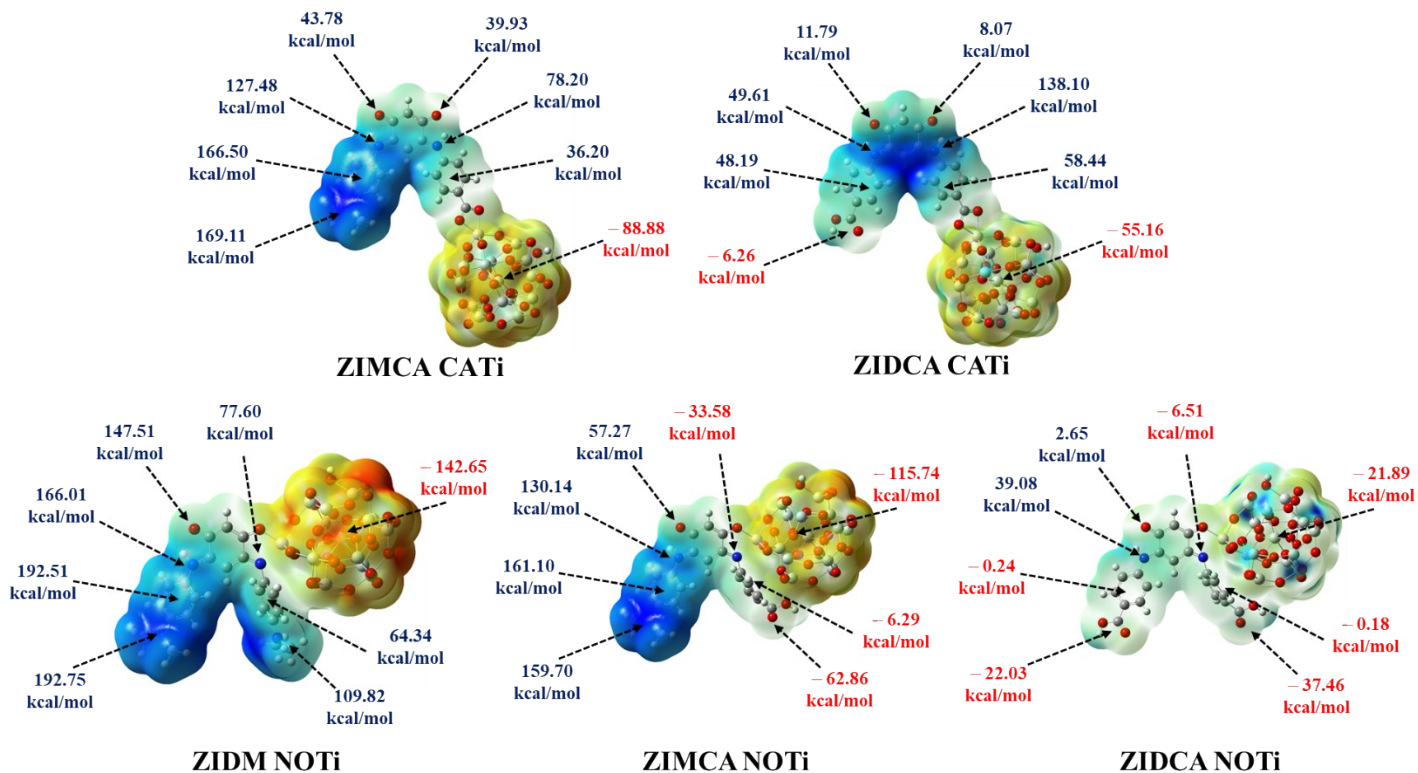
[suryapratap412@gmail.com](mailto:suryapratap412@gmail.com), [chy16sj.sharma@pg.ictmumbai.edu.in](mailto:chy16sj.sharma@pg.ictmumbai.edu.in) (S. J. Sharma)

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SI Fig. 2 MEP plots of ZIDM@TiO<sub>2</sub>, ZIMCA@TiO<sub>2</sub>, and ZIDCA@TiO<sub>2</sub> with NOTiO<sub>2</sub> and CATiO<sub>2</sub> binding modes

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Dyes	Phase	$E_{ox}^{dye}$	$E_{ox}^{dye*}$	$\Delta E$	$\Delta G_{inject}$	$\Delta G_{reg}$	LHE	$V_{oc}$
		(eV)	(eV)	(eV)	(eV)	(eV)	-	(eV)
ZIDM	Gas	6.67	4.39	2.28	0.39	1.87	0.0041	2.56
	DCM	6.71	4.39	2.32	0.39	1.91	0.2084	2.17
ZIMCA	Gas	7.00	4.82	2.18	0.82	2.20	0.0014	2.06
	DCM	6.91	4.63	2.28	0.63	2.11	0.1364	1.91
ZIDCA	Gas	7.32	5.21	2.11	1.21	2.52	0.0002	1.66
	DCM	7.54	5.26	2.27	1.26	2.74	0.0064	1.69

SI Table 2 Computed  $\Delta G_{inject}$ ,  $\Delta G_{reg}$ , LHE, and  $V_{oc}$  of ZIDM, ZIMCA, and ZIDCA optimized at DFT and TD-DFT results of  $\omega$ B97XD/6-311++G (d, p) level of theory

Dyes	Phase	$E_{ox}^{dye}$	$E_{ox}^{dye*}$	$\Delta E$	$\Delta G_{inject}$	$\Delta G_{reg}$	LHE	$V_{oc}$
		(eV)	(eV)	(eV)	(eV)	(eV)	-	(eV)
ZIDM	Gas	7.21	4.93	2.28	0.93	2.41	0.0016	3.17
	DCM	7.29	4.95	2.34	0.95	2.49	0.1457	2.78
ZIMCA	Gas	7.51	5.32	2.18	1.32	2.71	0.0002	2.71
	DCM	7.46	5.17	2.29	1.17	2.66	0.0863	2.53
ZIDCA	Gas	7.81	5.70	2.11	1.70	3.01	0.0007	2.35
	DCM	8.07	5.79	2.28	1.79	3.27	0.0039	2.33

