Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information (ESI)

Intermolecular Interactions between a Ru Complex and Organic Dyes in Cosensitized Solar Cells: A Computational Study

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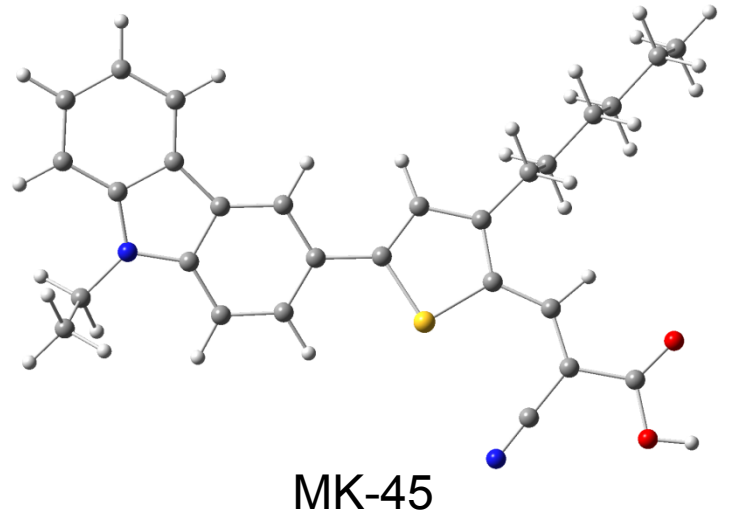
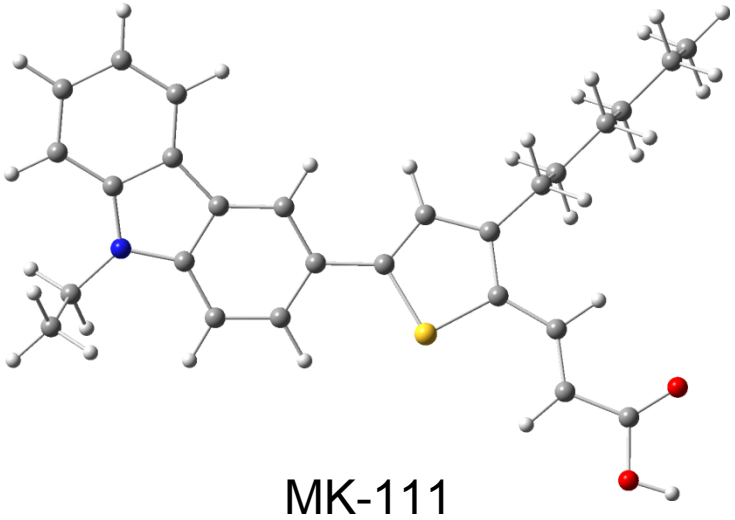


MK-45



MK-111

Fig. S1 Optimized geometries of the MK-45 and MK-111 monomers. White, grey, blue, red, and yellow indicate H, C, N, O, and S atoms, respectively.

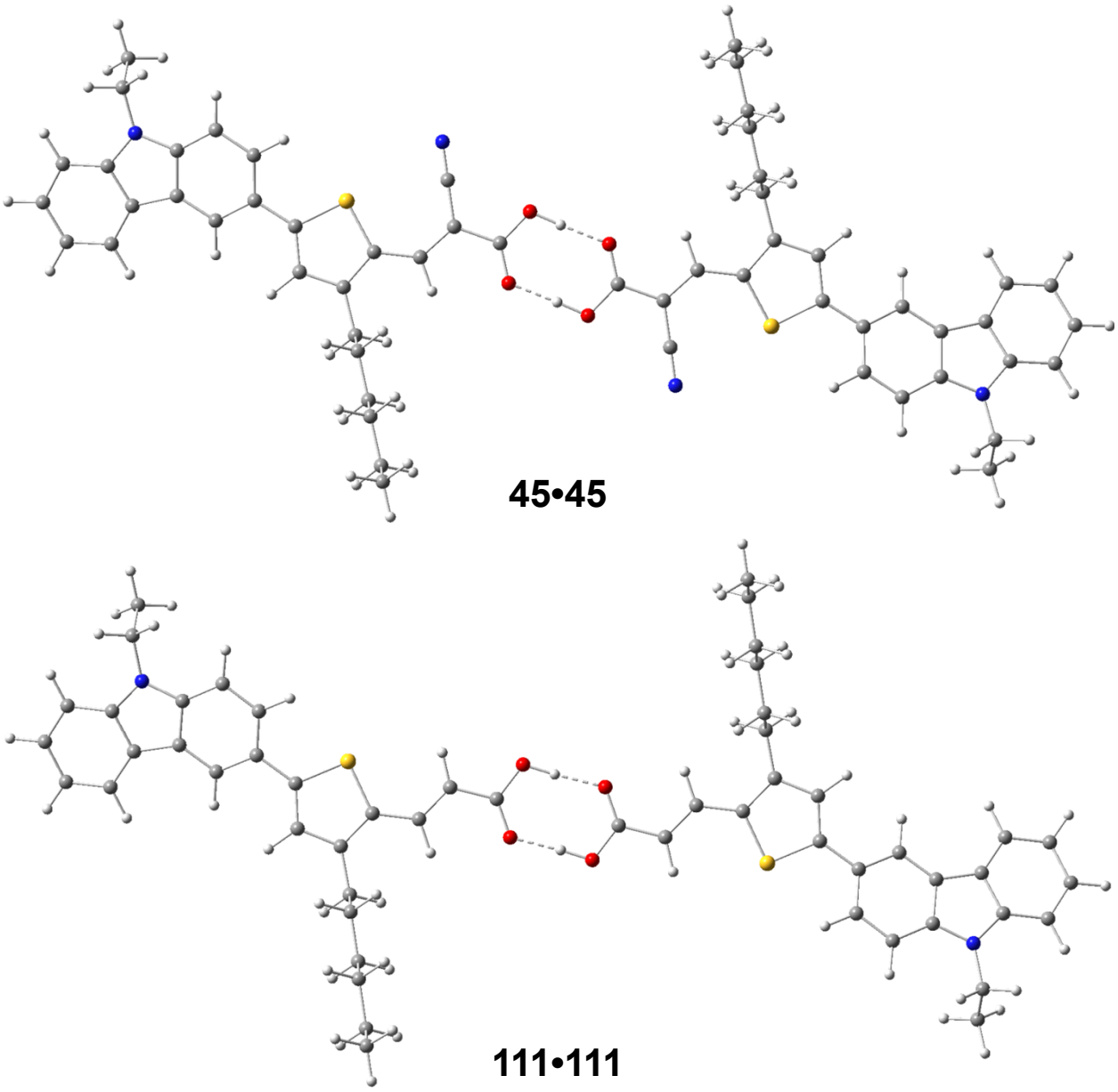
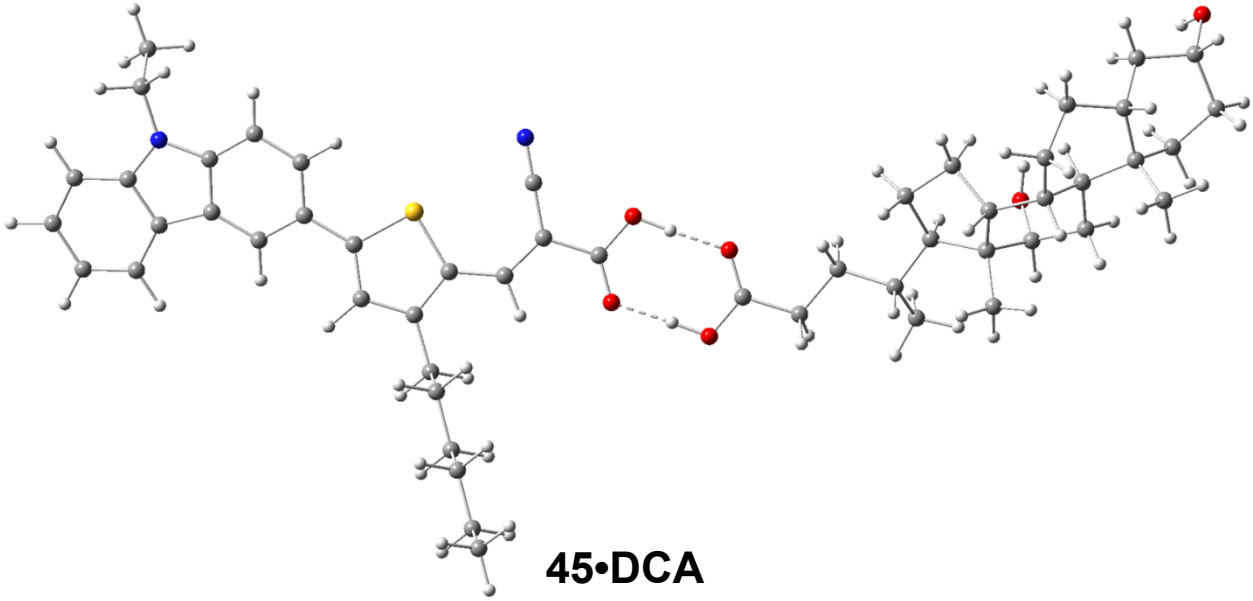


Fig. S2 Optimized geometries of the MK dimers. White, grey, blue, red, and yellow indicate H, C, N, O, and S atoms, respectively.



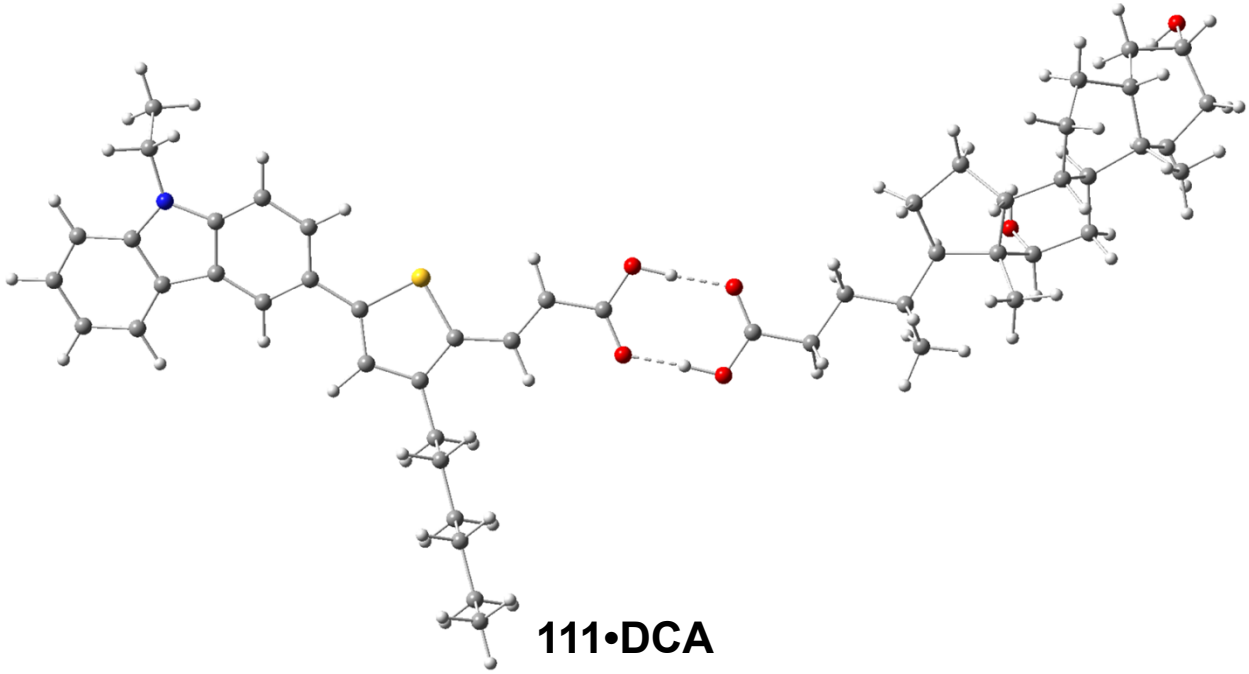


Fig. S3 Optimized geometries of the MK-45–DCA and MK-111–DCA species. White, grey, blue, red, and yellow indicate H, C, N, O, and S atoms, respectively.

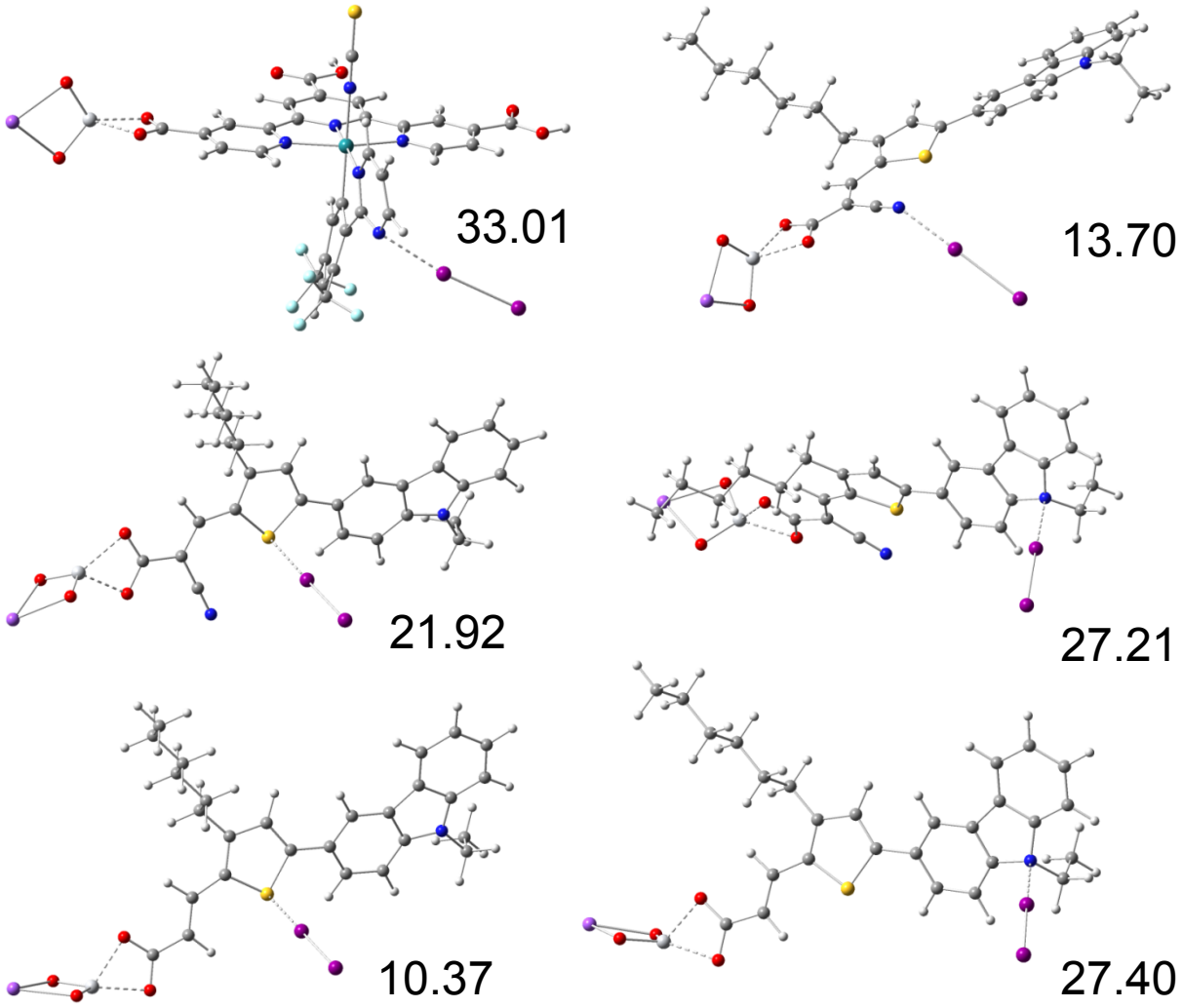


Fig. S4 Optimized geometries of the dye(TiO_2Na)–I_2 species with positive ΔG values. White, grey, blue, red, aqua, purple, yellow, ash, teal, and violet indicate H, C, N, O, F, Na, S, Ti, Ru, and I atoms, respectively. ΔG values are given in kJ mol^{-1}.

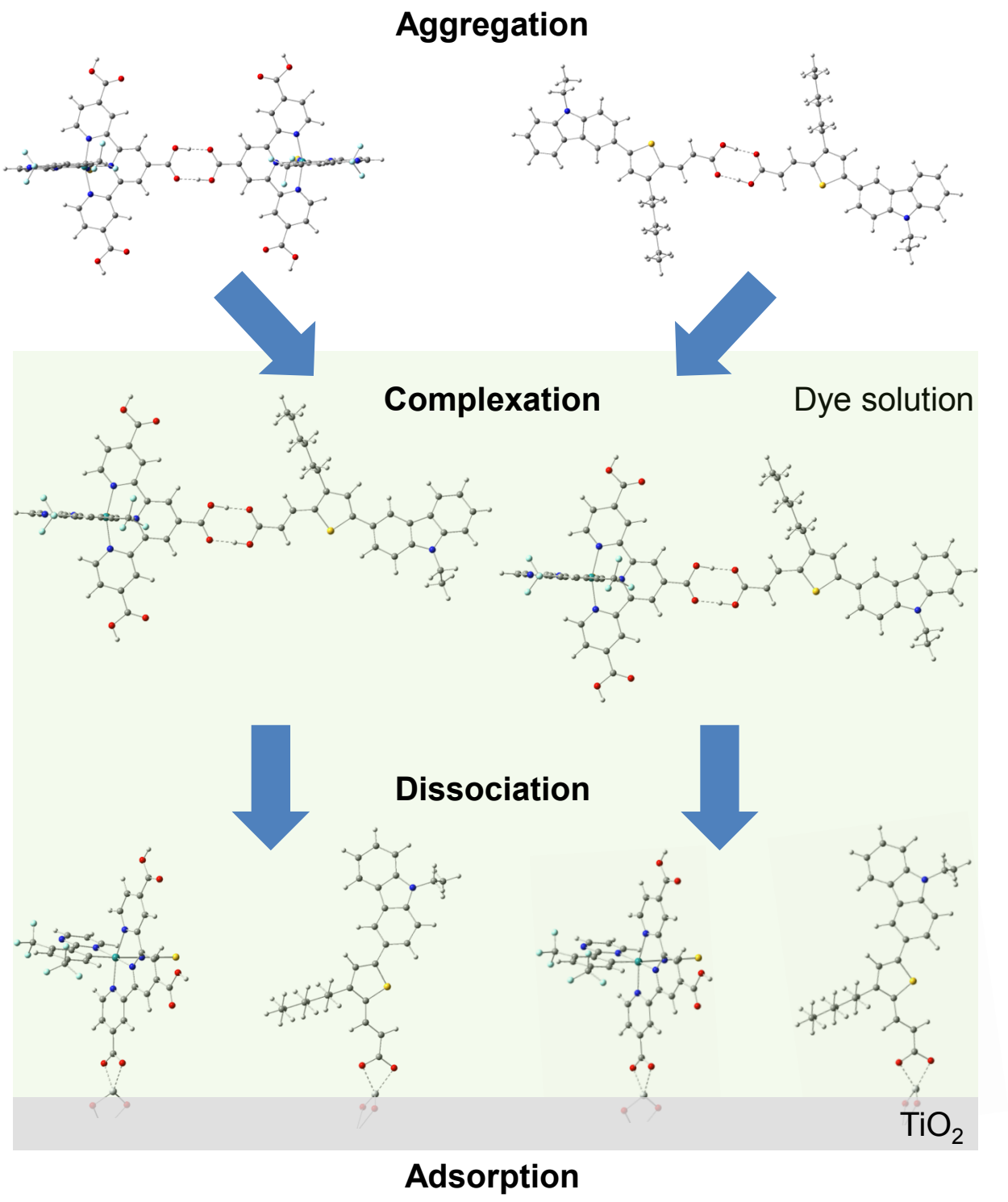


Fig. S5 Proposed suppression mechanism for FT89 aggregation by MK-111 during the immersion process of a TiO_2 film.

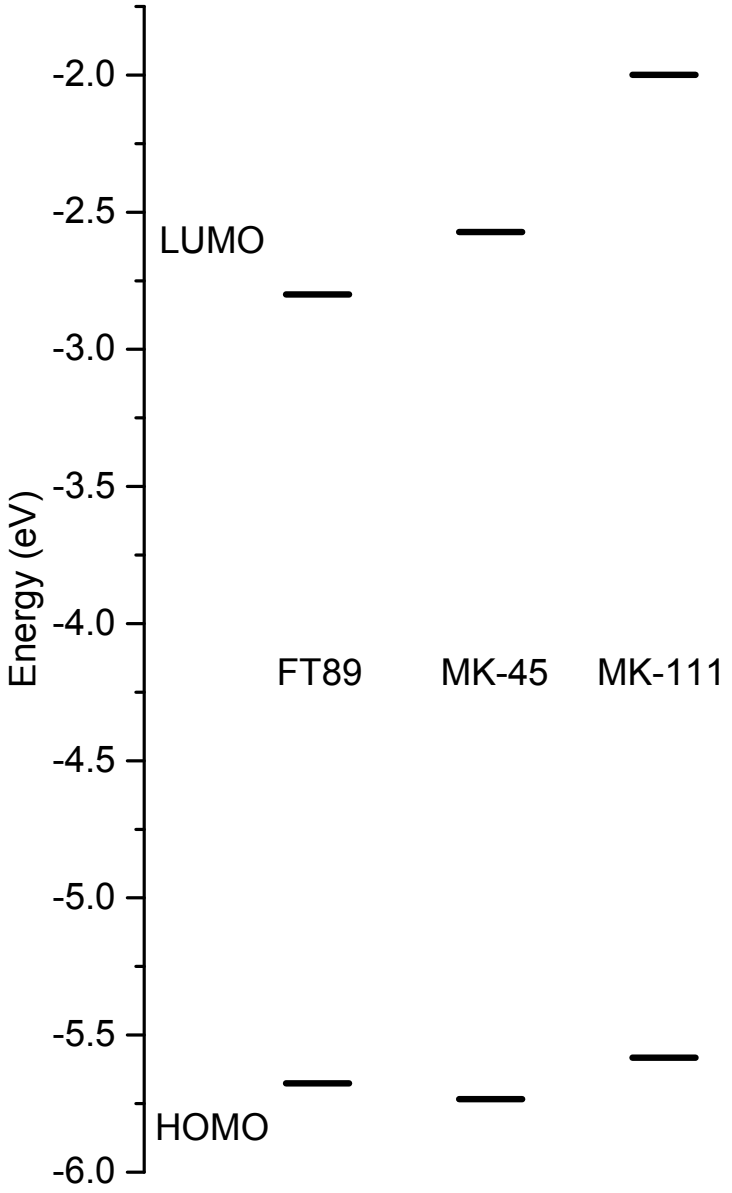


Fig. S6 Energy level diagrams of the dyes.

Table S1 Selected bond distances (Å) and dihedral angles (deg) for MK-45 and MK-111

	C–T distance	T–A distance	C–T dihedral	T–A dihedral
MK-45	1.456	1.411	160.0	–178.0
MK-111	1.460	1.430	156.9	–177.4

Table S2 Photovoltaic performances of DSSCs under 100 mW cm^{-2} of AM1.5G filtered light[S1]

Entry	Dye	J_{sc}[a] (mA cm^{-2})	V_{oc}[b] (V)	*ff*[c]	η[d] (%)	Γ[e] of FT89 (10^{-7} mol cm^{-2})	Γ[e] of MK dye (10^{-7} mol cm^{-2})
1	FT89	19.2	0.67	0.71	9.1	2.3	
2	MK-45	10.4	0.73	0.73	5.5		4.5
3	MK-111	6.8	0.68	0.72	3.4		4.3
4	FT89+MK-45	19.9	0.69	0.68	9.4	1.2	1.8
5	FT89+MK-111	21.0	0.71	0.66	9.8	1.0	2.0
6	FT89+DCA	20.5	0.70	0.67	9.6	1.6	
7	FT89+MK-45+DCA	20.7	0.70	0.69	10.0	1.4	1.3
8	FT89+MK-111+DCA	21.2	0.71	0.68	10.2	1.1	1.3

[a] Short-circuit photocurrent density. [b] Open-circuit photovoltage. [c] Fill factor. [d] Solar energy conversion efficiency. [e] Amount of sensitizer.

Notes and references

S1 T. Funaki, N. Koumura and K. Sayama, *Chem. Lett.*, 2013, **42**, 1371–1373.