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**Novel design of organic donor-acceptor dyes without carboxylic acid anchoring
groups for dye-sensitized solar cells**

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Table S1 Optical and electrochemical data of donor-acceptor dyes **1-4**.

	λ_{max} (nm [eV]) ^a	$E_{\text{ox},1}$ (V) ^b	$E_{\text{red},1}$ (V) ^b	HOMO (eV) ^c	LUMO (eV) ^c
1 ^{S1}	570 [2.18]	+0.86	-0.69	-5.66	-4.11
2 ^{S2}	759 [1.63]	+0.42	-0.50	-5.22	-4.30
3 ^{S3}	600 [2.07]	+0.85	-0.62	-5.65	-4.18
4 ^{S3}	750 [1.65]	+0.64	-0.49	-5.44	-4.31

^a In CH₂Cl₂.

^b In CH₂Cl₂ containing 0.1 M (nC₄H₉)₄NPF₆. Potential vs. Fc/Fc⁺.

^c Determined by $E_{\text{ox},1}$ and $E_{\text{red},1}$ under the assumption of Fc/Fc⁺ = -4.8 eV.

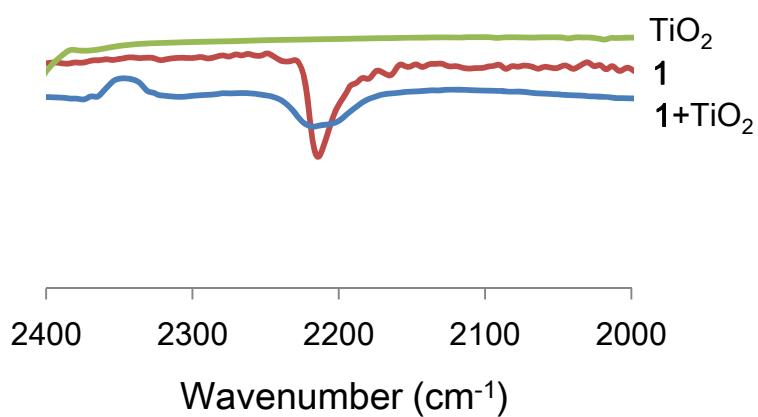


Fig. S1 IR spectra of TiO₂, **1**, and **1** adsorbed on TiO₂.

References

- S1 T. Michinobu, J. C. May, J. H. Lim, C. Boudon, J.-P. Gisselbrecht, P. Seiler, M. Gross, I. Biaggio and F. Diederich, *Chem. Commun.*, **2005**, 737.
- S2 M. Kivala, C. Boudon, J.-P. Gisselbrecht, P. Seiler, M. Gross and F. Diederich, *Chem. Commun.*, **2007**, 4731.
- S3 X. Tang, W. Liu, J. Wu, C.-S. Lee, J. You and P. Wang, *J. Org. Chem.*, **2010**, 75, 7273.