

Electronic Supplementary Information (ESI)

Efficient Metal-free Sensitizers Bearing Circle Chain Embracing π -Spacer for Dye-sensitized Solar Cells

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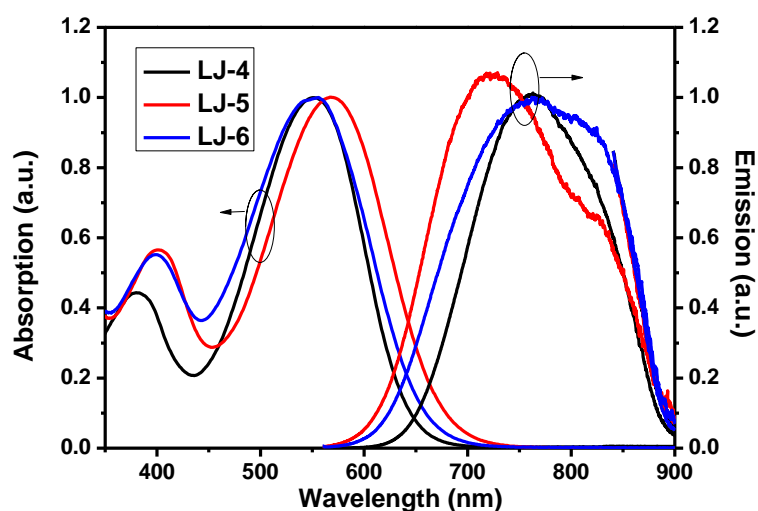


Fig. S1 Normalized UV-vis and emission spectra of dyes LJ-4, LJ-5 and LJ-6 in CH_2Cl_2 .

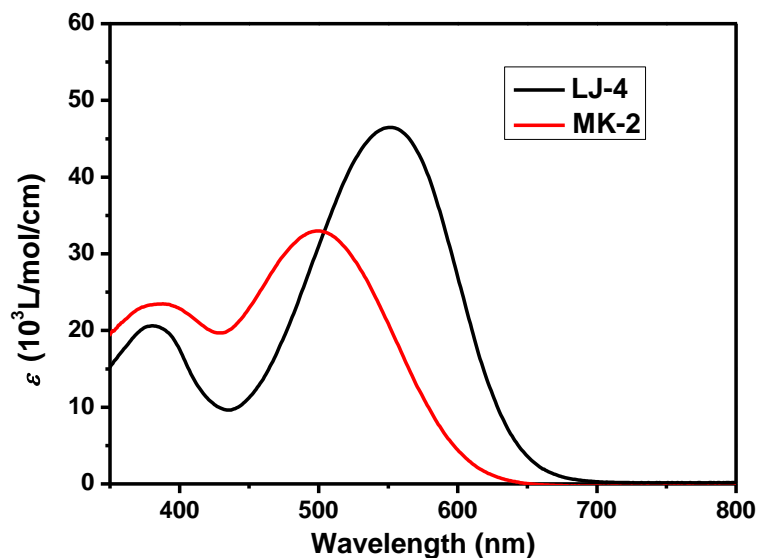


Fig. S2 UV-vis spectra of dyes LJ-4 and MK-2 in CH_2Cl_2 (2×10^{-5} M)

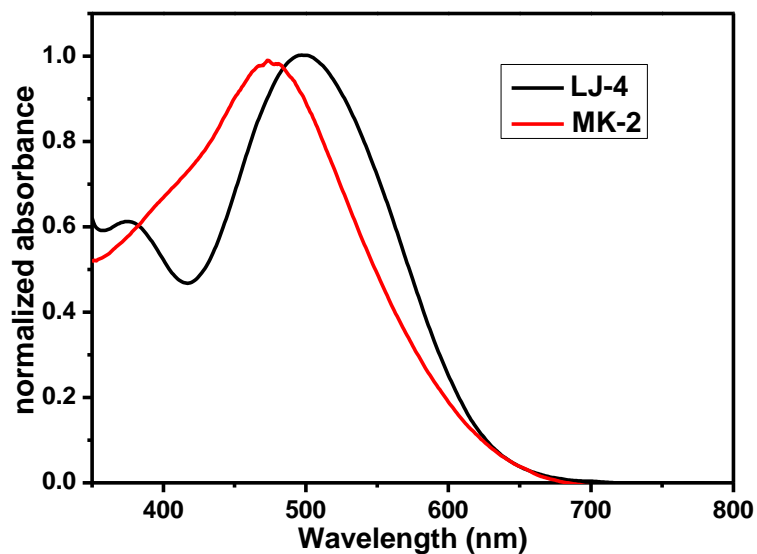


Fig. S3 Normalized UV-vis spectra of dyes **LJ-4** and **MK-2** anchored on TiO₂ film.

DFT Calculation

Geometry optimization and Molecular orbital distributions of three dyes were performed using B3LYP functional and 6-31G (d,p) basis set implemented in the Gaussian 09 program package.¹

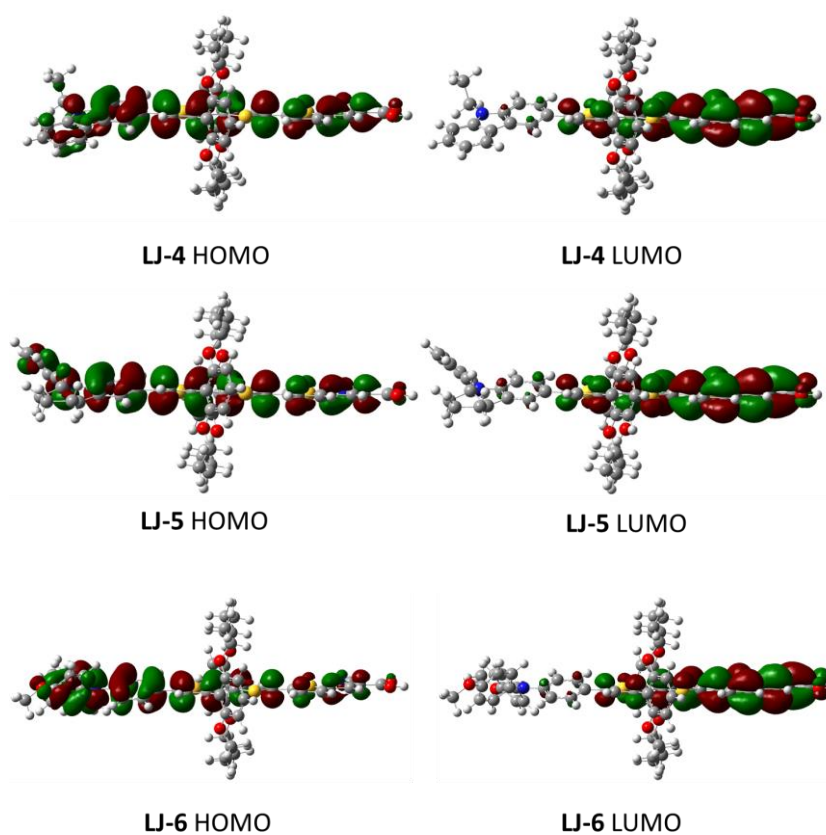


Fig. S4 The HOMO and LUMO of dyes **LJ-4**, **LJ-5** and **LJ-6** optimized at B3LYP/6-31G** level.

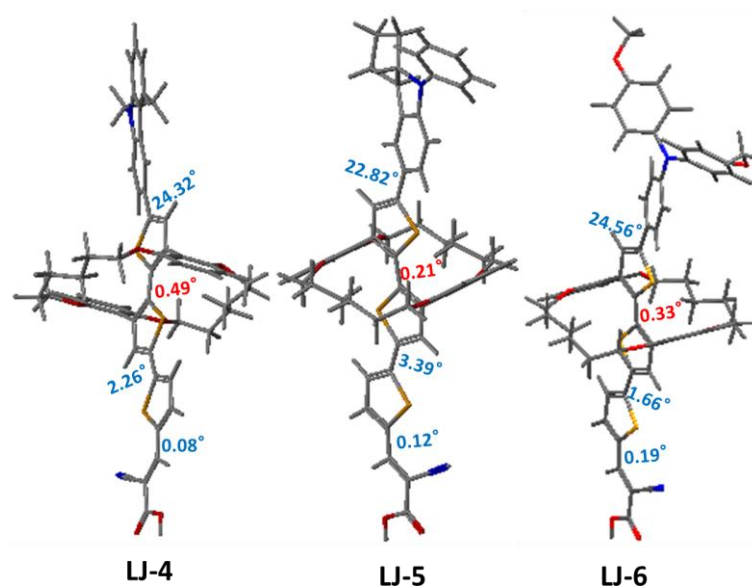


Fig. S5 Optimized ground-state geometries and dihedral angles between the π -planes of **LJ-4**, **LJ-5** and **LJ-6**.

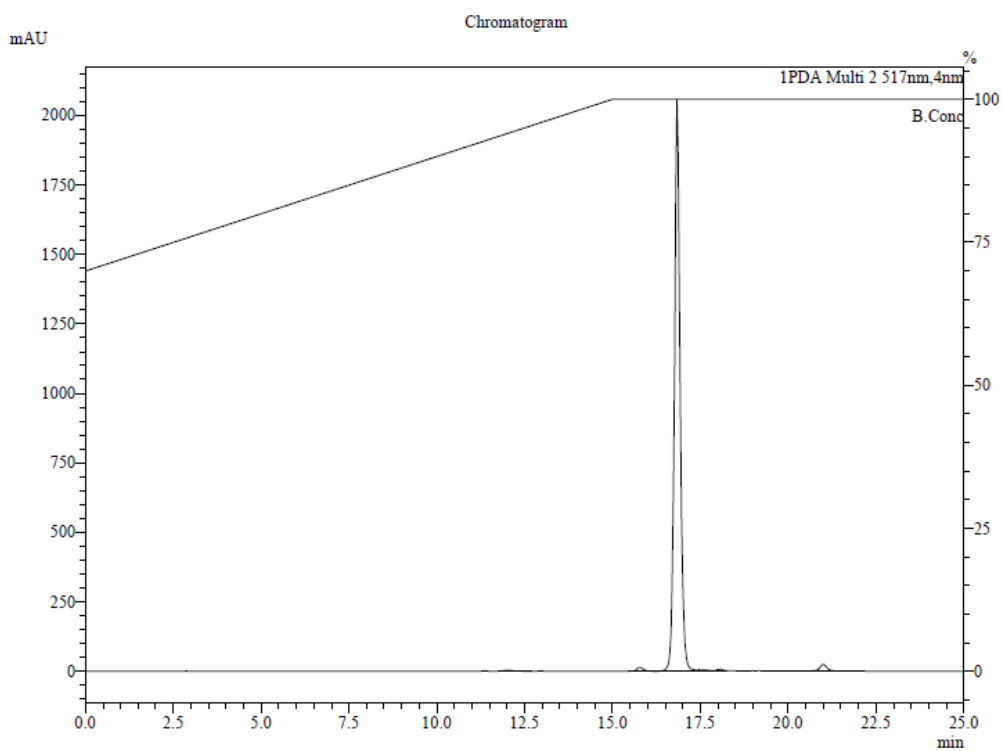


Fig. S6 HPLC analysis of dye **LJ-4** (purity: 97.8%); mobile phase A: 1% formic acid in water; mobile phase B: acetonitrile, gradient program: B: 70% (0 min)→ B: 100% (15-30 min).

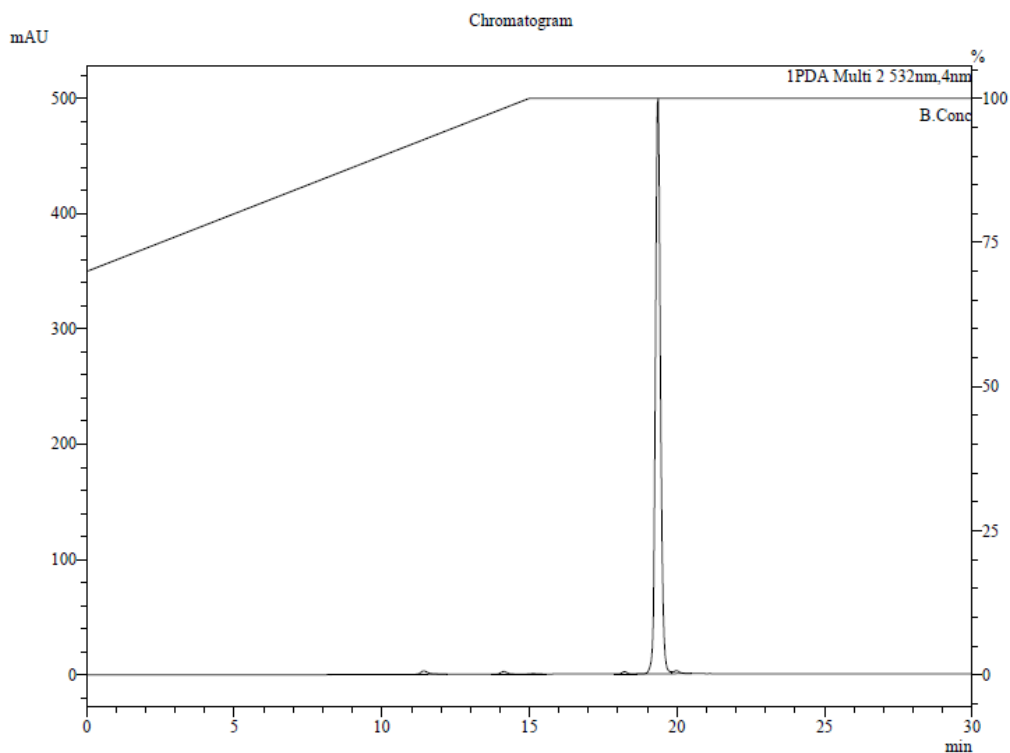


Fig. S7 HPLC analysis of dye **LJ-5** (purity: 97.8%); mobile phase A: 1% formic acid in water; mobile phase B: acetonitrile, gradient program: B: 70% (0 min)→ B: 100% (15-30 min).

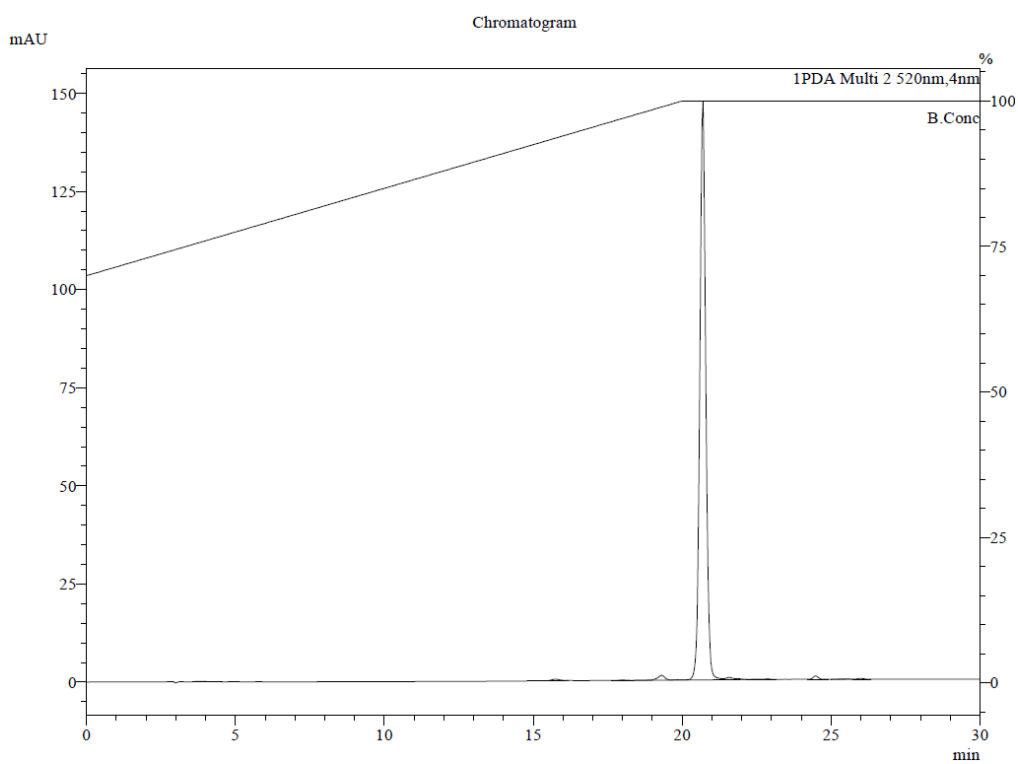


Fig. S8 HPLC analysis of dye **LJ-6** (purity: 97.8%); mobile phase A: 1% formic acid in water; mobile phase B: acetonitrile, gradient program: B: 70% (0 min)→ B: 100% (15-30 min).

Reference

1. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian 09, Revision A.02; Gaussian, Inc.: Wallingford, CT, **2009**.