# Supporting Information for

## Enhanced photovoltaic performance by synergism of light-cultivation and electronic localization for highly efficient dye-sensitized solar cells

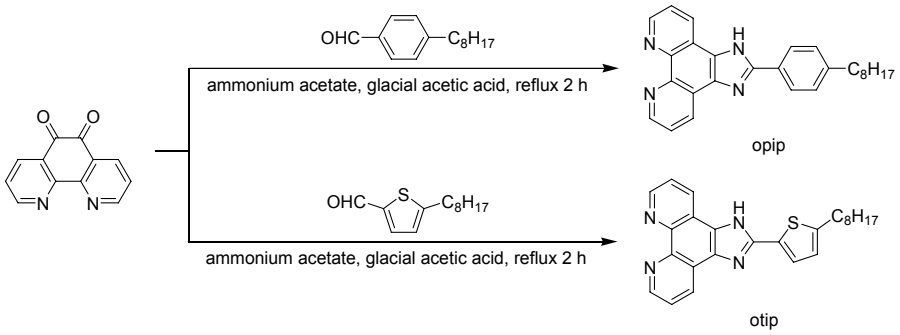
**Jen-Fu Yin,[a] Dibyendu Bhattacharya,[b] Ying-Chan Hsu,[b] Chen-Chuan Tsai,[b] Kuang-Lieh Lu,*[b] Hong-Cheu Lin,*[a] Jian-Ging Chen[c] and Kuo-Chuan Ho[c]**

[a] *Department of Materials Science and Engineering, National Chiao Tung University, Hsinchu 300, Taiwan*
[b] *Institute of Chemistry, Academia Sinica, Taipei 115, Taiwan. Fax: 886-2-27831237; Tel: 886-2-27898518; E-mail: lu@chem.sinica.edu.tw*
[c] *Department of Chemical Engineering, National Taiwan University, Taipei 106, Taiwan*

# 1. Experimental section

## (1) Synthesis of ligands opip and otip

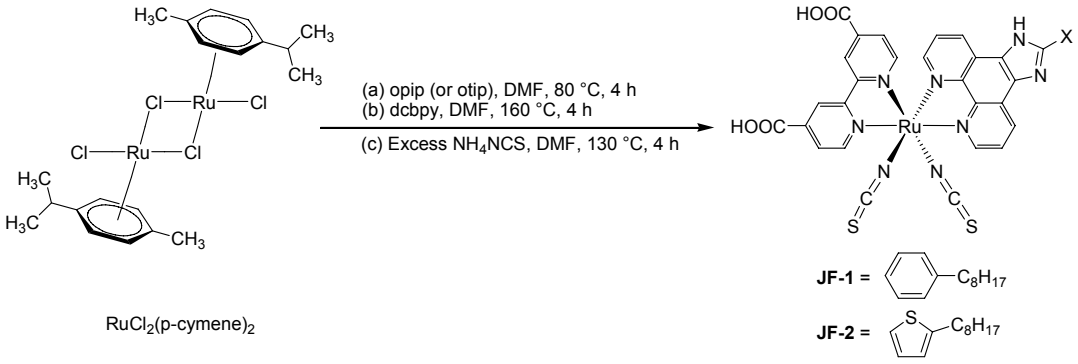
The synthetic procedure of opip and otip are showed in Scheme S1.




**Scheme S1.** Synthesis of ligands opip and otip.

## (2) Synthesis of ruthenium sensitizers JF-1 and JF-2

The one-pot synthetic procedure developed for heteroleptic polypyridyl ruthenium complexes was employed for the preparation of new sensitizers **JF-1** and **JF-2**. The synthetic procedure of **JF-1** and **JF-2** were showed in Scheme S2.




**Scheme S2.** Synthesis of ruthenium sensitizers **JF-1** and **JF-2**.

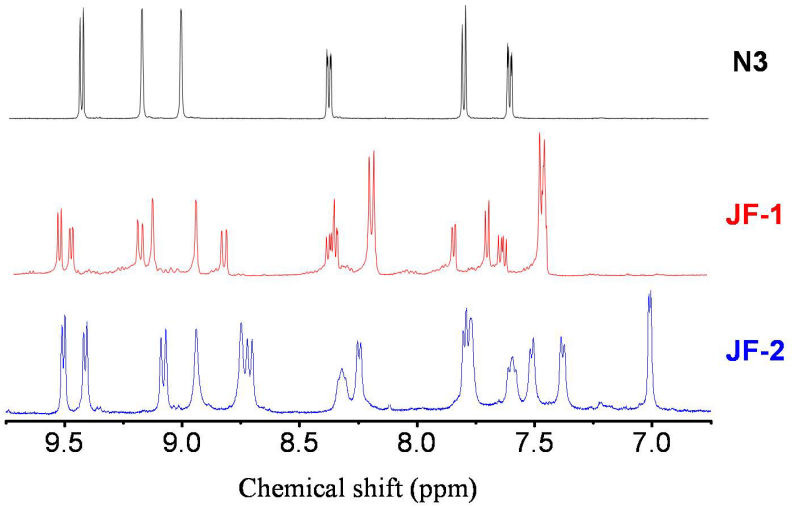



**Fig. S1** $^{1}$H-NMR spectrum (aromatic region) of **N3**, **JF-1** and **JF-2** in $d_6$-DMSO.

## 2. The spectra mismatch factor (M)

The deviation in power-conversion efficiency can be calculated from the spectra mismatch factor (M) using equation 1,

$$M = \frac{\int_{\lambda_1}^{\lambda_2} E_R(\lambda) S_R(\lambda) d\lambda \int_{\lambda_1}^{\lambda_2} E_S(\lambda) S_T(\lambda) d\lambda}{\int_{\lambda_1}^{\lambda_2} E_R(\lambda) S_T(\lambda) d\lambda \int_{\lambda_1}^{\lambda_2} E_S(\lambda) S_R(\lambda) d\lambda} \qquad (1)$$

where $E_R(\lambda)$ is the reference spectral irradiance, $E_S(\lambda)$, the source spectral irradiance, $S_R(\lambda)$, the spectral responsivity of the reference cell, and $S_T(\lambda)$, the spectral responsivity of the cell that was fabricated by us. In this instance, we used a Si reference solar cell (Oriel 91150, calibrated by the National Renewable Energy Laboratory (NREL) as the reference cell.

## 3. The UV-vis absorption and emission spectra of opip and otip

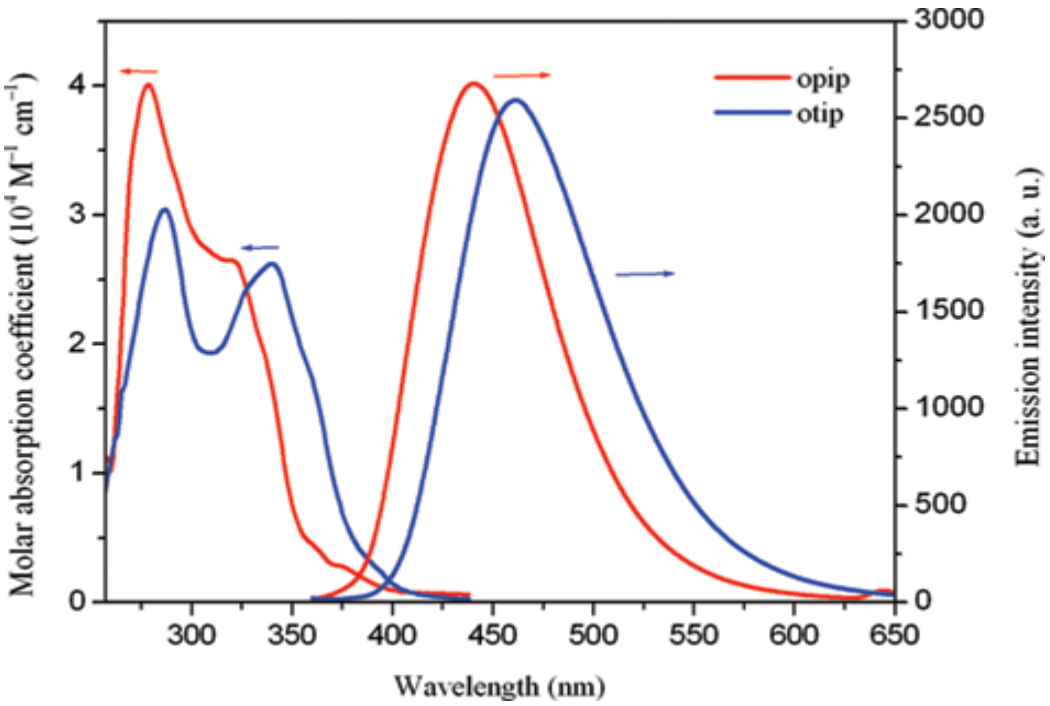



**Fig. S2** UV-vis absorption and emission spectra of the free ligands, opip and otip, in DMF.

## 4. Computational selected bond lengths [Å] and angles (deg) of complexes JF-1 and JF-2

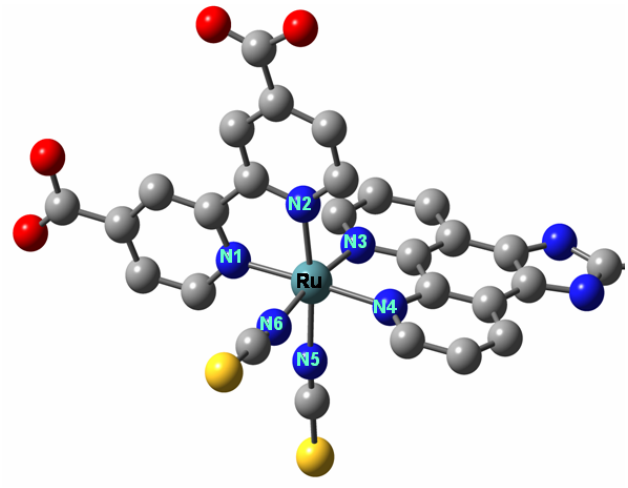



**Fig. S3** Structural schematic diagrams of **JF-1** and **JF-2** for atom numbering.

**Table S1** Selected bond distances [Å] and angles [deg] of complexes **JF-1** and **JF-2** in calculated singlet ground-state geometry using the DFT at the B3LYP/LanL2DZ level.

| Compound | Ru–N1 | Ru–N2 | Ru–N3 | Ru–N4 | Ru–N5 | Ru–N6 | N1–Ru–N4 | N2–Ru–N5 |
|---|---|---|---|---|---|---|---|---|
| **JF-1** | 2.02 | 2.01 | 2.03 | 2.04 | 2.05 | 2.05 | 177.97 | 173.13 |
| **JF-2** | 2.04 | 2.05 | 2.07 | 2.07 | 2.06 | 2.05 | 177.30 | 172.18 |

## 5. Relative frontier molecular energy level diagram of complexes JF-1 and JF-2

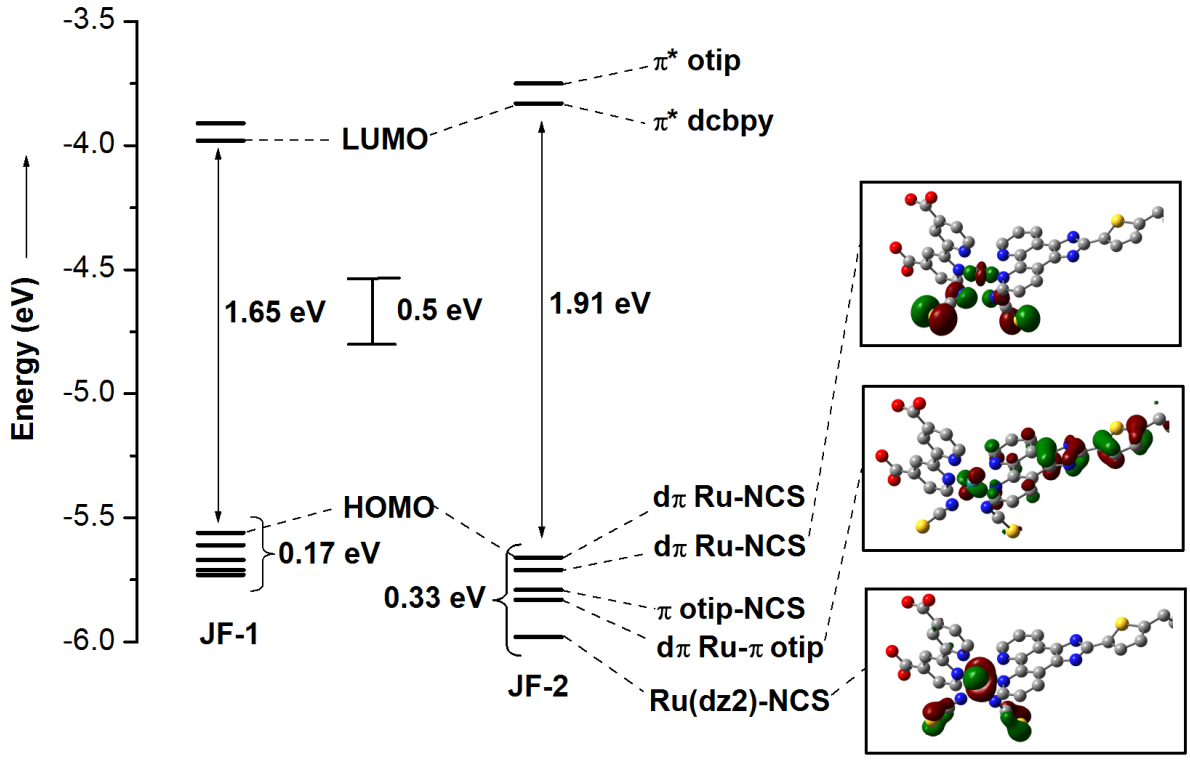



**Fig. S4** Energy and character of the frontier MOs of **JF-1** and **JF-2**. Also shown are isodensity plots of selected MOs. For better clarity on the major components in the MOs, we set isovalue = 0.04 for these plots.