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Electronic Supplementary Information

Breaking aggregation in a tetrathiafulvalene-fused zinc porphyrin by metal-ligand coodination to form a donor-acceptor hybrid for ultrafast charge separation and charge stabilization

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1. Supplementary Figures

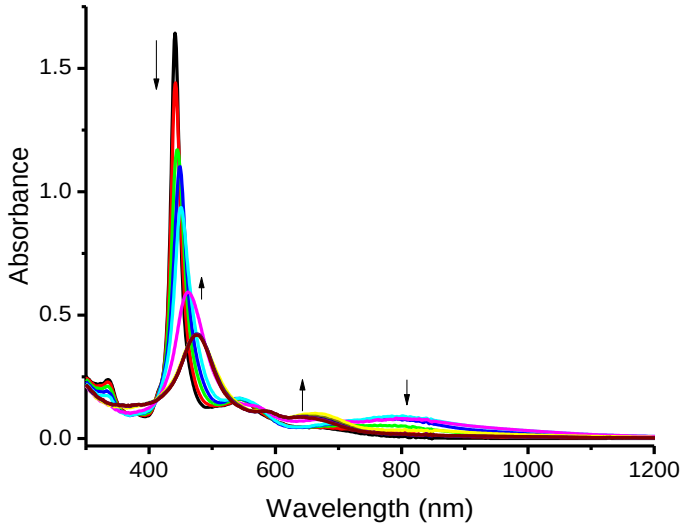

Fig. S1. Absorption spectral changes observed during increased addition of nitrosonium hexafluoroantimonate (0.2 equivalent each addition) to a solution of $(TTF)_4PZn$ in DCB.

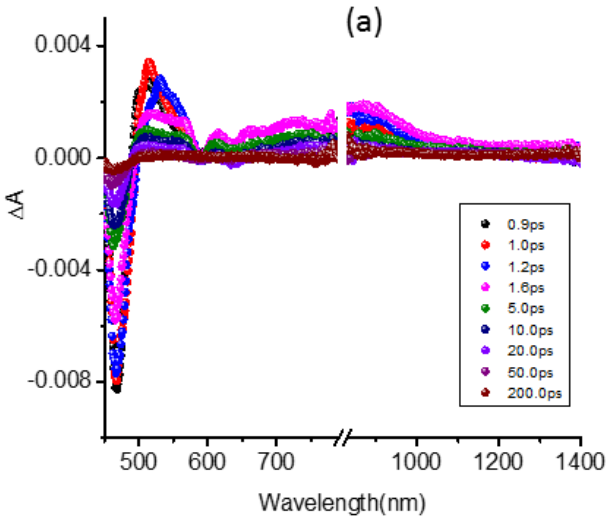

Fig. S2. Femtosecond transient absorption spectrum of $(TTF)_4PZn$ at the indicated time intervals in DCB.

2.0 Characterization data for $(TTF)_4PH_2$ and $(TTF)_4PZn$

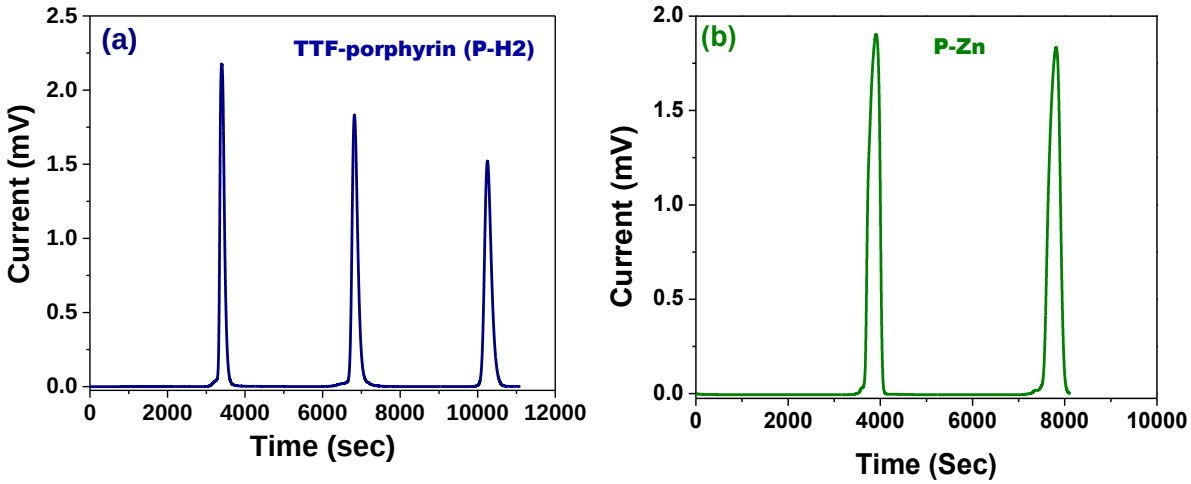

Fig. S3. Partial HPLC-GPC traces for the free base $(TTF)_4PH_2$, (a); and its corresponding Zn(II)-complex, $(TTF)_4PZn$, (b) used in this study.

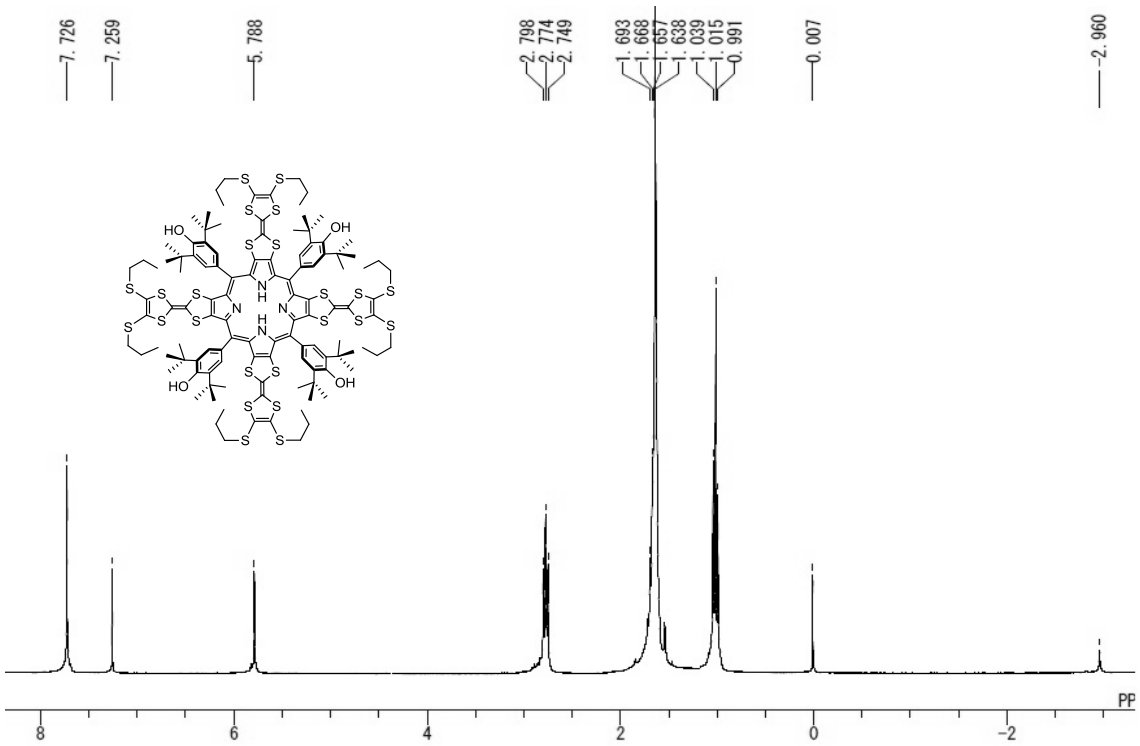

Fig. S4. ^{1}H NMR spectrum (300 MHz) of $(TTF)_4PH_2$ recorded in $CDCl_3$ at 298 K.

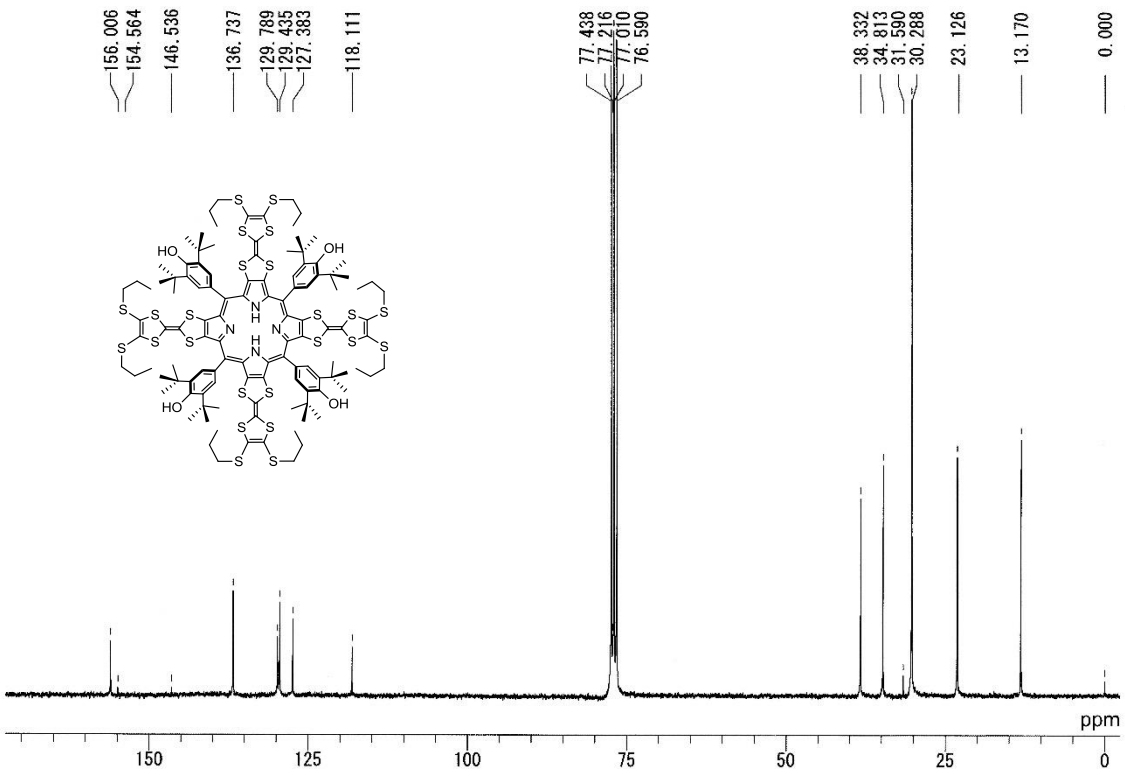

Fig. S5. ^{13}C NMR spectrum (75 MHz) of $(TTF)_4PH_2$ recorded in $CDCl_3$ at 298K.

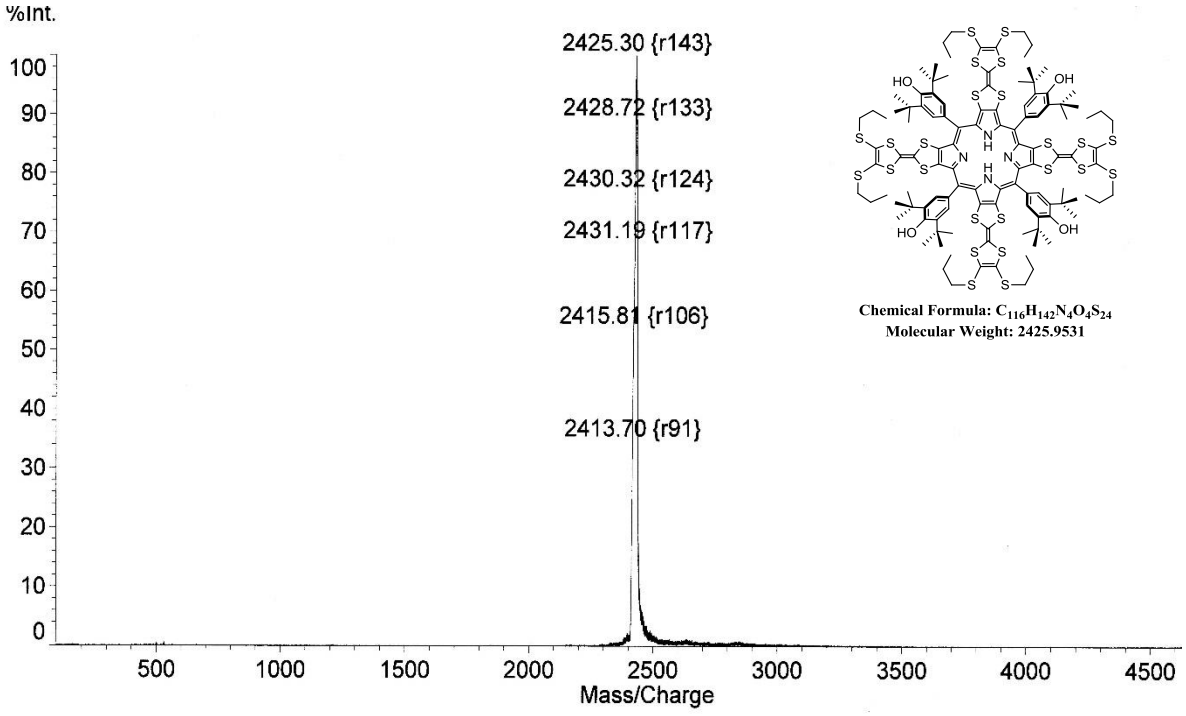

Fig. S6. MALDI-TOF mass spectrum of $(TTF)_4PH_2$.

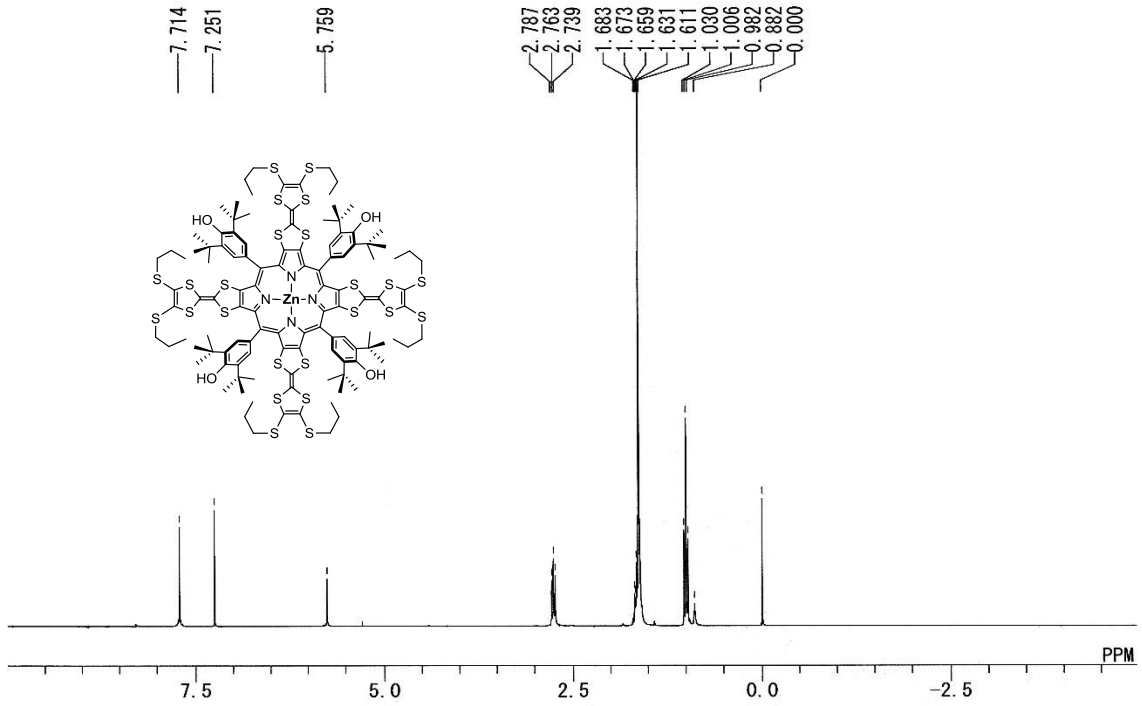

Fig. S7. ^{1}H NMR spectrum (300 MHz) of $(TTF)_4PZn$ recorded in $CDCl_3$ at 298 K.

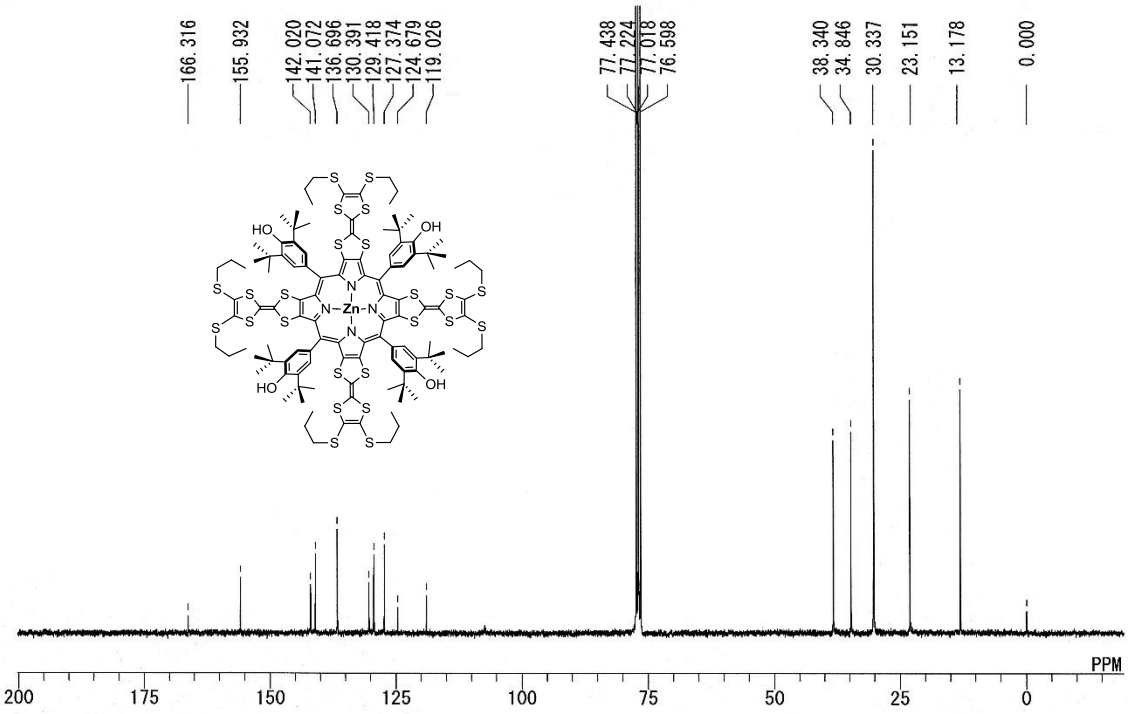

Fig. S8. ^{13}C NMR spectrum (75 MHz) of $(TTF)_4PZn$ recorded in $CDCl_3$ at 298 K.

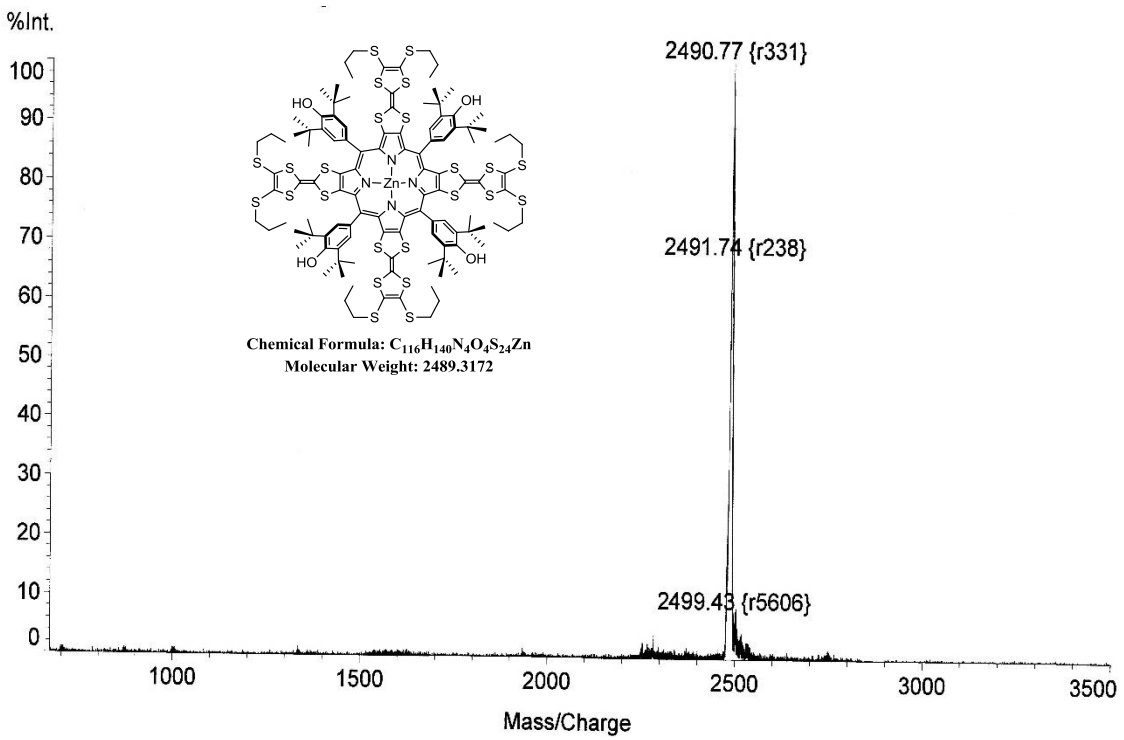

Fig. S9. MALDI-TOF mass spectrum of $(TTF)_4PZn$.

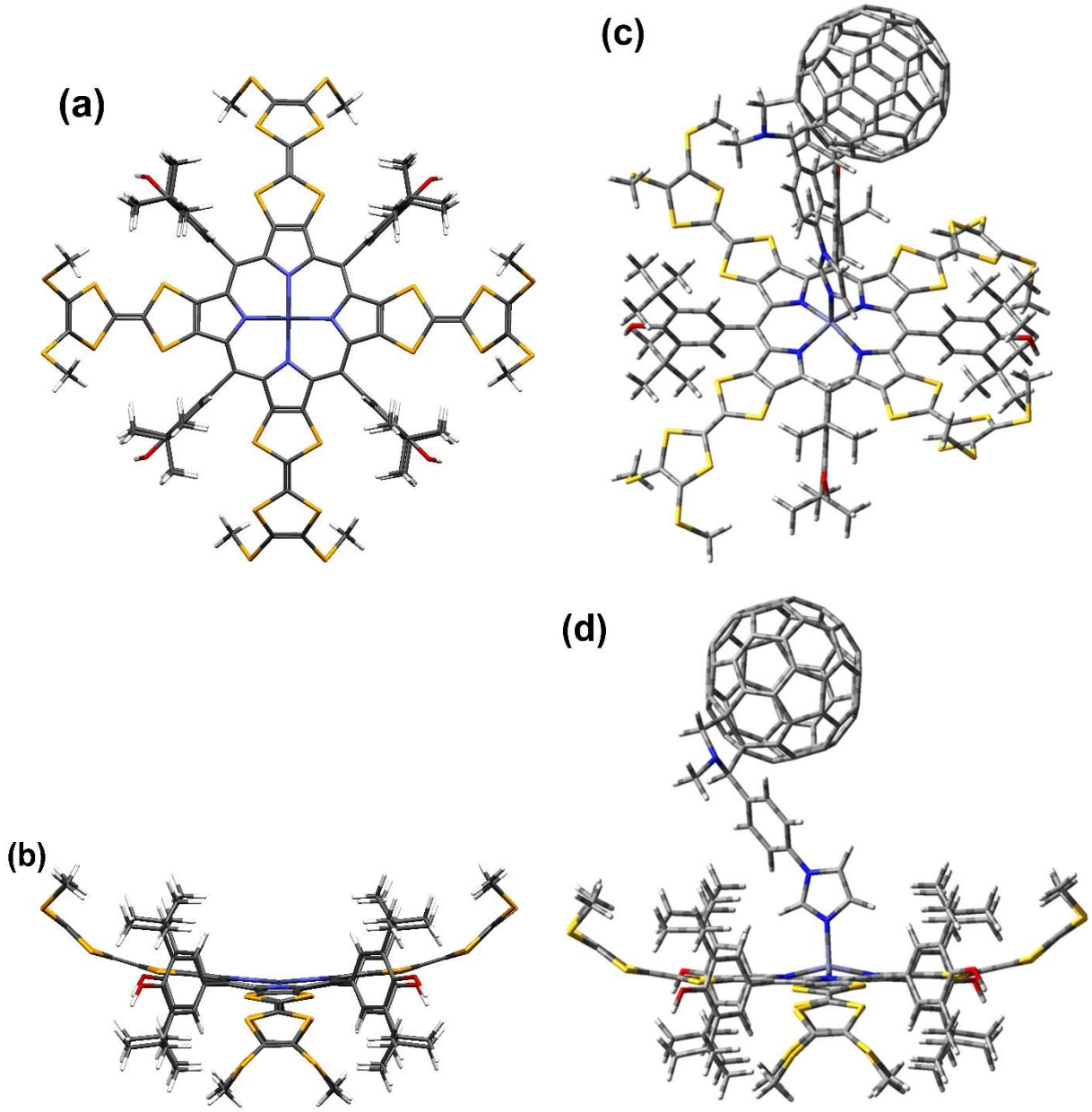

Fig. S10. Optimized geometry of the $(TTF)_4PZn$, (a) top view, (b) side view along with its supramolecular dyad $(TTF)_4PZn:C_{60}Im$; (c) top view, (d) side view, respectively.

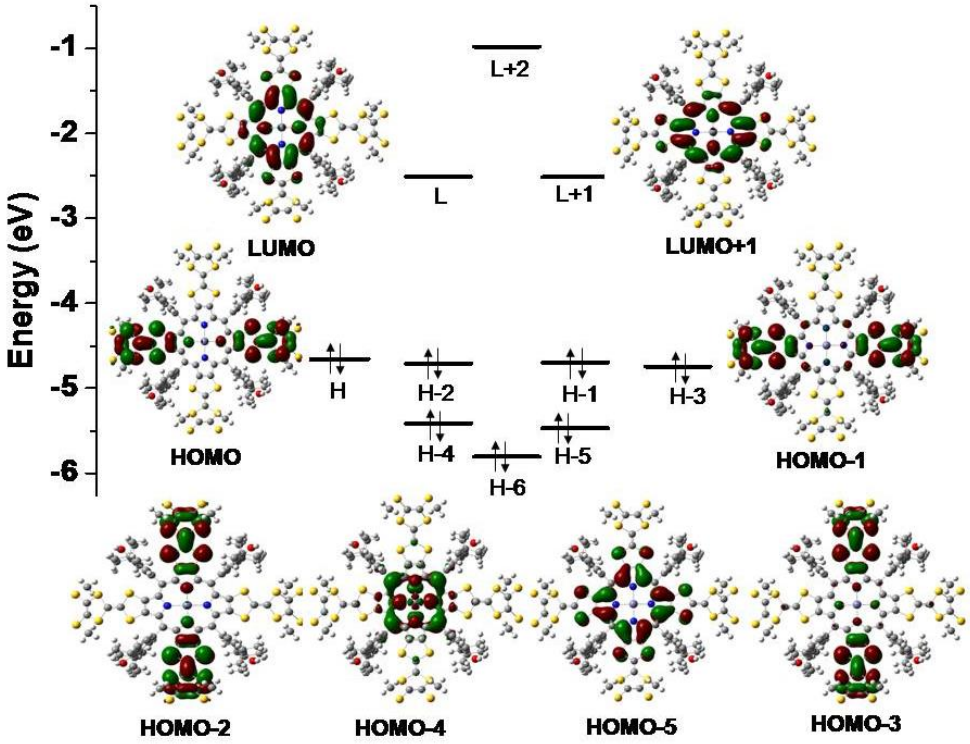

Fig. S11. Molecular Orbital (MO) energy diagram for $(TTF)_4PZn$**.**

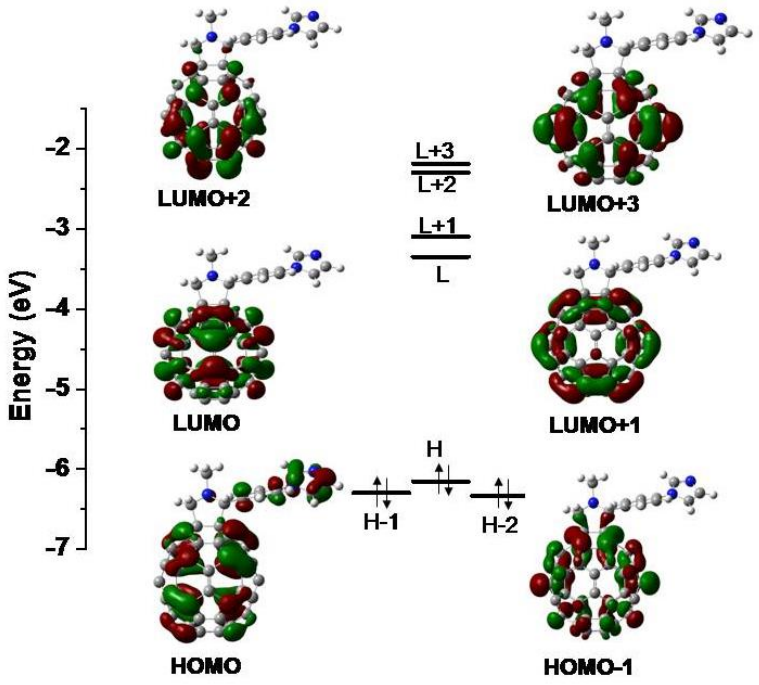

Fig. S12. Molecular Orbital (MO) energy diagram for C_{60}Im.

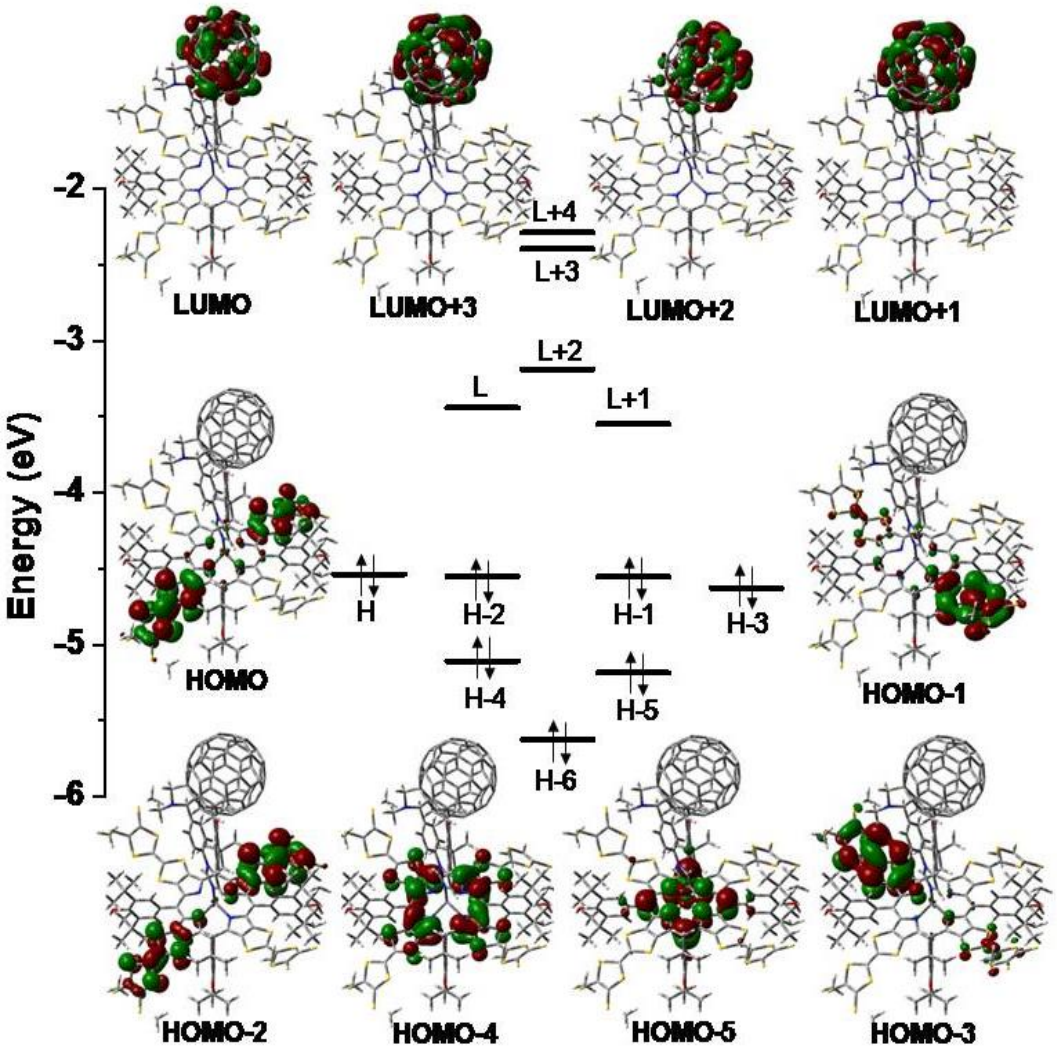

Fig. S13. Molecular Orbital (MO) energy diagram for the supramolecular dyad $(TTF)_4PZn:C_{60}Im$ used in this study.