Theoretical studies on POM-based organic-inorganic hybrids containing double D-A1-π-A2 chains for high performance p-type dye-sensitized solar cells (DSSCs)

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ELECTRONIC SUPPLEMENTARY INFORMATION

S1. Theoretical background for p-type DSSCs

As we known, there are five dominating steps in the work of p-type DSSCs, which are shown in following:

$Dye|NiO + h\nu \rightarrow Dye^{*}|NiO$ (excitation) (1)

$Dye^{*}|NiO \rightarrow Dye^{-}|NiO + h^{+}(NiO)$ (hole injection) (2)

$Dye^{-}|NiO + h^{+}(NiO) \rightarrow Dye|NiO$ (geminate recombination) (3)

$Dye^{-}|NiO + 1/2\ I_3^{-} \rightarrow Dye|NiO + 3/2\ I^{-}$ (dye regeneration) (4)

$3/2\ I^{-} \rightarrow 1/2\ I_3^{-} + e^{-}(Pt)$ (I_3^{-} regeneration) (5)

The first step is the dye excitation by light absorption and immediately followed by the hole injection from excited dye into the valence band of the semiconductor. However, if the reduced dye can't react with electrolyte within the charge-separated lifetime, it may recombine with the hole in semiconductor (the third step). Next, the dye is regenerated by electron transfer from the reduced dye to the oxidized species (I_3^{-}) in electrolyte. Finally, the holes in semiconductor move to the back collector of working electrode and the reduced species (I^{-}) in electrolyte diffuses to the Pt electrode.

S2. Molecular orbital diagrams for systems **I** and **II0** involved in the dominant electron transitions

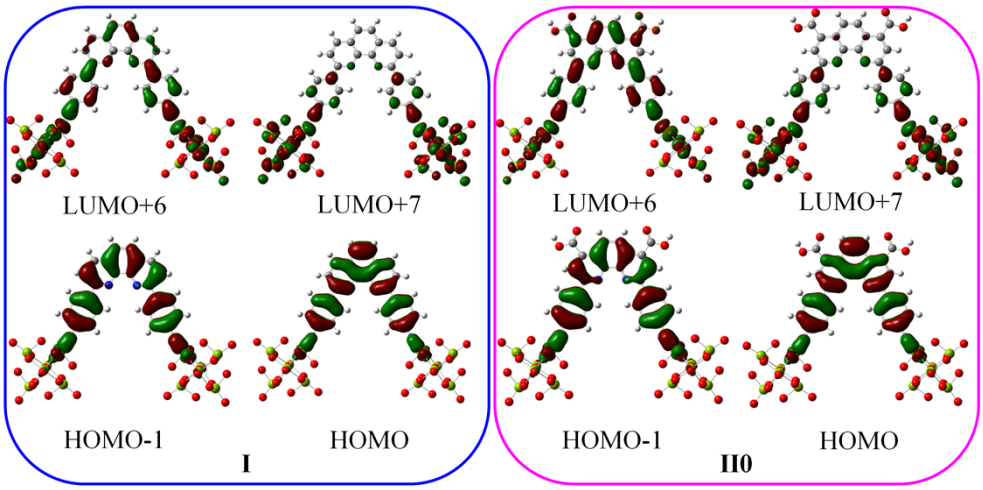

Fig. S2 Molecular orbital diagrams for systems **I** and **II0** involved in the dominant electron transitions