Efficient DSCs with Preciously Tunable Energies and High Open-circuit Voltage Enabled by Organic Molecular Engineering

Dye sensitized solar cells (DSCs) have attracted much research attention due to their promise in facile fabrication process and low-cost conversion of solar energy. A common DSC consists of a dye sensitizer and TiO_2 electron acceptor that work together to convert light to electricity. Although intense research attention had been focused on the dye molecule, systematic study on the importance of the energy levels of the dyes has merely been reported. Generally, the electrochemical properties of a dye are determined by the Lowest Unoccupied Molecular Orbital (LUMO) levels and Highest Occupied Molecular Orbital (HOMO) levels, which is related to and charge injection into the TiO_2 and dye regeneration after charge injection, respectively. Recently reported by Graetzel, *et al* show that the copper compound-based electrolyte can efficiently regenerate dyes with minor potential driving force, and thus DSSCs based on copper electrolyte generally exhibit high V_{OC} and good efficiency. However, due to the low-lying HOMO level of the copper-based electrolytes, the dye molecules shall have suitable reducing potential for efficient dye regeneration.

Our work on a series of IDT based organic dyes prove that the large coplanar conjugated IDT core can lower-down the HOMO level of the dye molecules matching with the low-cost copper electrolyte, $Cu^{I/II}(tmby)_2TFSI$. On the other hand, via control over the electron accepting part, we found perfectly matching energy levels of the dyes and electrolytes for both charge injection and dye regeneration, as well as proper UV-Vis absorptions for the IDT based dyes, enabling efficient DSSCs with ~11% efficiency and ~1.2 V voltage.

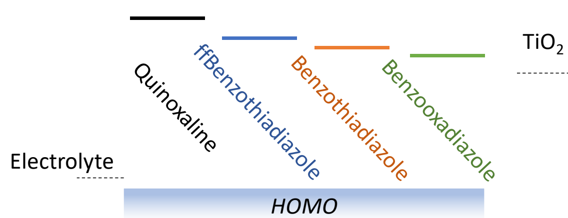

Figure 1. Energy Diagram of the Organic Dyes.

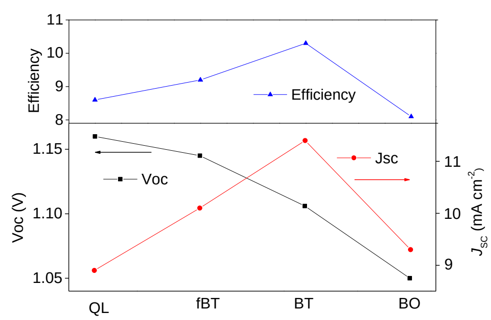

Figure 2. Summary of the Efficiencies, V_{OC} and J_{SC} of the IDT Dyes-Based DSSCs.

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