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Accessing the Charge Separation Effects in Dye-Sensitized Solar Cells Based on a Vectorial Planning of Supramolecular Ruthenium Dyes

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Abstract

Charge recombination has been postulated a critical point in dye sensitized solar cells (DSSC), however the role of the electron-hole separation distance from the TiO₂ surface and the oxidized dye has actually never been experimentally demonstrated for this type of device, operating under normal working conditions. In order to elucidate this point, supramolecular ruthenium dyes encompassing vectorial electron transfer properties have been especially devised, consisting of electronically coupled [Ru(dcbH₂)₂(B)Cl]⁺ and [Ru(dmb)₂(B)Cl]⁺ complexes acting as acceptor-donor pairs, respectively, where dcbH₂= 2,2'-bipyridine-4,4'-dicarboxylic acid, and dmb= 4,4'-dimethyl-2,2'-bipyridine. In these systems, the two ruthenium complexes are connected by linear bridging ligands (B) of programmed lengths, e.g. 1.85, 2.06 and 2.70 nm for 4,4'-bipyridine (bpy), *trans*-1,2-bis(4-pyridyl)-ethylene (bpe) or *trans*-1,4-bis[2-(4-pyridyl)ethenyl]-benzene (bpeb), respectively, thus allowing a precise control of the interfacial charge-separation distance. By working under similar, reproducible conditions, the overall efficiency of the corresponding DSSCs increased from 2.78 (bpy) to 2.89 (bpe) and 3.25% (bpeb), paralleling the increase of the bridging ligand lengths. Such results were corroborated by impedance measurements, highlighting the important role of the electron-hole separation effect in DSSCs, and also demonstrating how a suitable supramolecular design can improve the overall cell efficiency.

Keywords: Solar Cells ; Supramolecular Chemistry • Charge Recombination; Binuclear Ruthenium Dyes; TiO₂ Devices

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