CONFIGURATION FOR DYE-SENSITIZED SOLAR CELLS

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Introduction. The conformation of the dye on the semiconductor is an important factor for the improvement of charge injection and minimization of the back electron transfer process. In addition, the dye should be able to suppress aggregation by introducing bulky alkyl groups, addition of co-adsorbents, or designing a dye with a π-bridge between two chromophores forming a spiro-like configuration [1,2]. This study presents the synthesis of two compounds having double D-TT-A configurations namely, KS-11 and KS-13 and comparing their photovoltaic properties with the rod-like configuration, herein labelled as KS-10.

Materials and methods. The syntheses of the dyes are according the synthetic route presented in the references with modifications. Dyes are soaked in 0.3 mM solutions in 1:1 DMSO/MeCN for 12 hours. The electrolyte consists of 0.7 M BMII, 0.05 M I_2, 0.02 M LiI, 0.5 M 4-tBP in MeCN/3-methoxypropionitrile. Photovoltaic measurements were obtained using a sealed cell under illumination of AM 1.5 with 0.159 cm^{-2} masking area using Oriel Sol3A solar simulator. Theoretical calculations for the free dyes were done using density functional theory with Gaussian 09 software and the dye-TiO_2 geometries were done using SCC-DFTB.

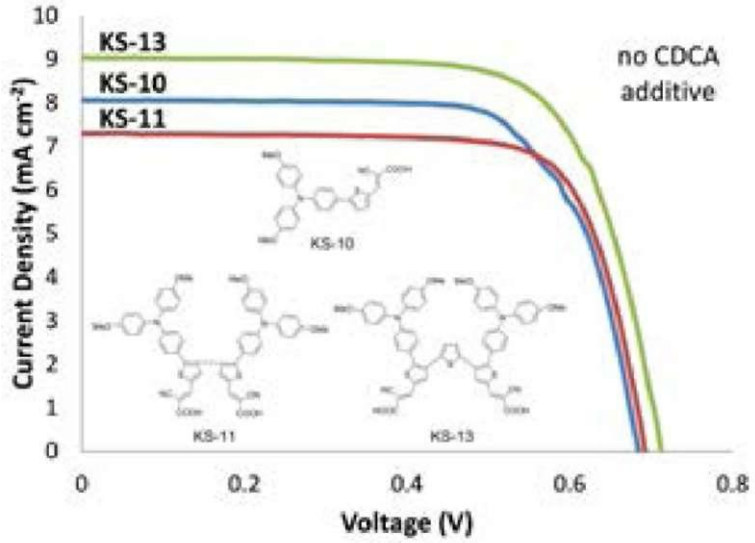

Figure 1. PV curves for DSSCs based on KS-10, KS-11, and KS-13

Results and discussion. Two double D-TT-A branched organic dye linked at the thiophene bridge were designed and synthesized for DSSCs. Their photophysical, electrochemical, and photovoltaic properties were investigated. As compared to the reference dye isomer containing a single D-TT-A branch, the double D-7T-A branched dye isomer consisting of two separated light-harvesting moieties in one molecule are beneficial to photocurrent generation provided that they are properly separated not to introduced exciton annihilation, as shown with the results. A 17 % increase in conversion efficiency was achieved in double D-TT-A branched organic dye as compared to the reference dye under simalated AM1.5G solar irradiation.

Conclusions. We have synthesized KS-10, KS-11, and KS-13 and based on the results, KS-13 has a better PV performance compared to KS-10 and KS-11. This is probably due to the stronger binding to the TiO_2 surface. The larger surface area of KS-13 also has the capacity to block efficiently the electrolyte.

References.

1. R. Sirohi, D.H. Kim, S.-C. Yu, S.H. Lee. *Dyes Pigm.* 92 (2012) 1132.
2. Y. Hong, J.-Y. Liao, D. Cao, X. Zang, D.-B. Kuang, L. Wang, H. Meier, C-Y. Su. *J. Org. Chem.* 76 (2011)8015.