

UNDERSTANDING AND CONTROLLING ELECTRON TRANSFER BETWEEN SENSITIZER AND ELECTROLYTE

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(This his Abstract is for an oral presentation to be delivered by Mr. Christopher P Kershaw)

The efficiencies of dye-sensitized solar cells (DSSC) have been increasing recently, with a recent high of 14.7%.¹ However, a pressure to develop devices with higher efficiencies has meant less research has gone on to understanding dye processing. One operational process is slow electron transfer between the reduced electrolyte and oxidised dye, which limits overall device performance.^{2,3} Previous work has suggested a sulphur atom can aid such processes. However, there is less detail on the role of sulphur and little evidence has been published to date.⁴

We have designed an experiment using modified half-squaraines to investigate the effects of co-sensitization and how the role of sulphur atoms and their position within dye sensitizers can affect device performance and lifetime.

Additionally, we have used the sulphur atom in these dyes as an atomic probe to study dye orientation at TiO₂ surfaces using angle-resolved X-ray photoelectron spectroscopy (AR-XPS). Using these data in conjunction with density functional theory (DFT) calculations of dye energy levels (e.g. HOMO and LUMO) and preferred dye orientations on model TiO₂ surfaces, we aim to obtain a deeper understanding of the electron transfer processes between the electrolyte and sensitizer. From this we will be able to optimise the surface structure of the photoelectrode in order to further optimise device performance and lifetime.

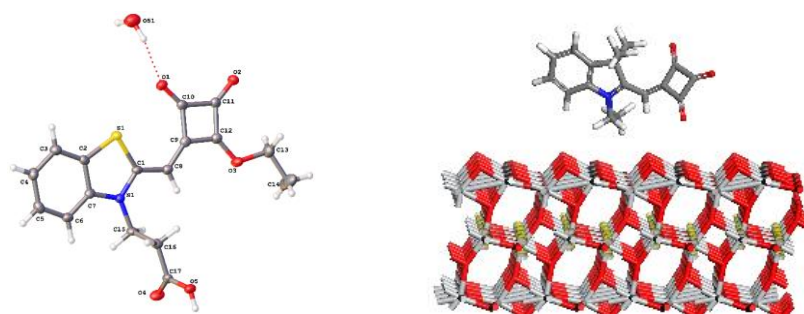


Fig. 1: (Left) Crystal structure of sulphur-containing half squaraine dye and (right) DFT studies of dye orientations on a TiO₂ surface

References

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