New Nitroxides Lift the Efficiency of Dye-Sensitised Solar Cells

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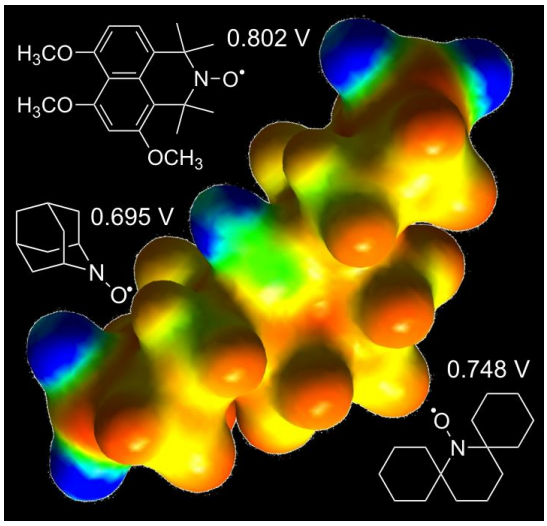
Major shortcomings of conventional solid-state solar cells - fragility, high cost and overheating - are overcome in the dye-sensitised solar cells (DSSCs), which, on top of that, display superior strength and flexibility and do not require full sunlight to afford reasonable efficiency. In a DSSC a so called 'redox mediator', typically the iodide/triiodide (I^-/I_3^-) pair, is required to transport an electron from counter electrode to the oxidised dye thus regenerating it. Unfortunately, the I^-/I_3^- mediator has a number of serious disadvantages, such as dark colour, corrosiveness and, most importantly, mismatch between its oxidation potential (0.35 V *vs* NHE) and that of a dye (*ca* 1.1 V), ultimately limiting lifespan and effectiveness of the cell. In contrast, redox mediators comprising a stable nitroxide radical/oxoammonium cation pair can potentially address these problems. In particular, their oxidation potentials are much closer to the optimal range of 0.60-0.85 V and can be easily manipulated by tailoring chemical structure of the mediator. Yet, the highest achieved efficiency of a solar cell utilizing nitroxide redox mediator (TEMPO in a Grätzel cell) [1] is only 5.4%, primarily due to the instability of the corresponding oxoammonium cation. Thus, there is a need for a nitroxide redox mediator that is stable, undergoes one-electron oxidation reversibly and has the potential in a desired range. We have employed high-level quantum chemical calculations to design nitroxides satisfying these criteria. We have considered over 100 different species and identified a number of successful candidates (see Figure) [2]. Following the publication of this work, experimental group in Japan has incorporated one of these promising nitroxides into a DSSC, which afforded an unprecedented energy conversion efficiency of 8.6% [3].



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