Are Most Organic DSC Dyes Photolabile?
Dye Photoisomerisation and Other Decay Paths

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The common design paradigm for organic DSC dyes involves Donor–π-brige–Acceptor/binding group and allows efficient charge flow from the donor to the acceptor and into the semiconductor. However, the π-linker also leads to excited state photochemistry, specifically double bond twisting. For two very important classes of organic DSC molecules, containing the cyanoacrylic acid and the rhodanine acceptor group, we show that photoisomerisation leads to a competitive process and a new isomer.[1,2] The most commonly used anchor, the cyanoacrylic binding group, undergoes photoisomerisation not just in solution, but also when the dye is adsorbed on a mesoscopic surface.[1] This process is therefore of relevance in complete cells and not only in dye solution.

Even highly efficient dyes like D149 and D102, containing the rhodanine acceptor group, are subject to photoisomerisation. The rather complicated photochemistry of these dyes also involves deactivation by protons, bound through hydrogen bonds, which significantly reduces the excited state lifetimes and competes with electron injection.[3] This excited state quenching by acids and protic solvents may be one reason for the increase in cell efficiency by bases such as benzimidazole.

Dye isomerisation is to be avoided, as it not only competes with electron injection but also as it may disrupt the surface structure and enable contact to the electrolyte. As a consequence, we suggest to prevent isomerisation by avoiding exocyclic double bond when designing new dyes.