Green organic dyes for DSSC application based on D-A-π-A design bearing Indigo structure

Daniele Franchi,[a,b] Massimo Calamante,[a,b] Alessandro Mordini,[a,b] Gianna Reginato,[b]
Lorenzo Zani,[b] Adalgisa Sinicropi.[c]

a) Università degli Studi di Firenze, Dipartimento di Chimica “Ugo Schiff”, Via della Lastruccia 13, 50019 Sesto Fiorentino (FI), Italy;
b) CNR - Istituto di Chimica dei Composti Organometallici (CNR-ICCOM), Via Madonna del Piano 10, 50019 Sesto Fiorentino (FI), Italy;
c) Università degli Studi di Siena, Dipartimento di Biotecnologie, Chimica e Farmacia, Via A. Moro 2, 53100 Siena, Italy;

Although dyes for DSSC capable of providing relatively high efficiencies have already been obtained and the path for improving the dye stability has already been undertaken, there are other issues which have been less investigated and need to be addressed. The new challenge in the field of building integrated photovoltaics is to complete the palette of colorations available for DSSCs. The development of libraries of dyes characterized not only by long-term stability and considerable high efficiency but also by a wide choice of colors, would make the exploitation of DSSCs much more appealing from an architectural point of view.

In this work, the preparation of near-IR absorbing green dyes is reported. The obtained compounds were spectroscopically and electrochemically characterized and the innovative dyes were employed to sensitize DSSC devices to evaluate their photo-electronic properties.

To design dyes possessing the desired coloration, we referred to D-A-π-A structures. With such design, a relatively small energy gap between the frontiers orbitals is predicted resulting in near-IR absorption. The dyes reported in this work (*Figure 1 right*) are characterized by Indigo internal acceptor. The peculiar blue coloration of Indigo structures is due to the cross-conjugated system of two electron-donating functions and two acceptors (the amines and the carbonyl functions respectively) known as H-Chromophore (*Figure 1 left*).

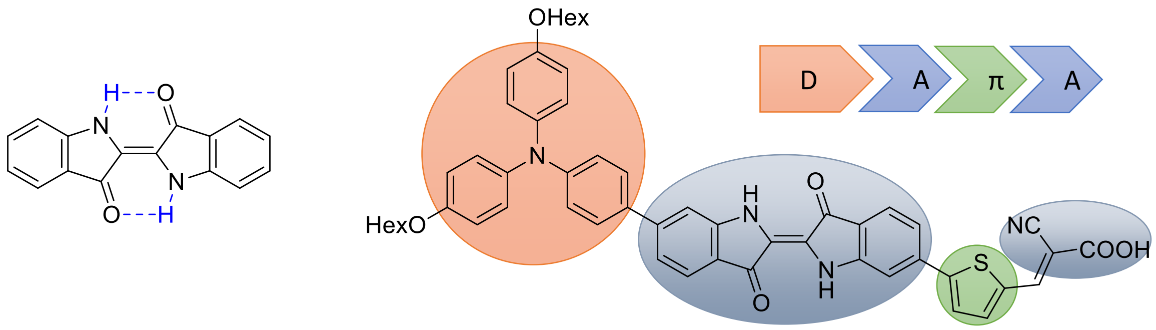

***Figure 1**: on the left-hand side the H-Chromophore is highlighted on the Indigo's structure. An example of a D-A-π-A dye bearing Indigo as the internal acceptor is reported on the right-hand side.*

The solubility issue of Indigo was solved with Boc protection of the amine. The elongation to the designed dyes was performed by means of palladium catalyzed cross-coupling reactions. Once the Boc protection was released the dyes displayed a good solubility and an interesting intense green coloration. Such feature was found to be the result of the combination of two absorption band one attributed to the charge transfer between the D-A moieties and the other one relative to the released Indigo’s H-Chromophore. The photo-electronic properties of the dyes, obtained from DSSC sensitized with the synthesized dyes, will be reported.