**Link:** <https://solar-power-tech.com/e-posters/dsc_eposter_01/>

**Abstract**

Basic photovoltaic parameters of the cells sensitized with a popular indoline D149 dye, containing carboxyl anchoring group, were compared with those of the cells sensitized with the dye modified by the addition of alkoxysilyl anchoring moiety [1].

The synthesis route was described using the popular indoline dye coded as D149 with its structure modified by the replacement of the anchoring group by alkoxysilyl (trimethoxysilyl) one. Application of two different types of electrolyte, based on iodide- and tris(2,2’-bipyridine)cobalt(II/III) redox couple (Co-Bpy), provided the information on long-term stability of DSSC systems, both with carboxyl- and alkoxysilyl groups. Our studies give the opportunity to better understand the dynamics of electron injection from the dye excited states to the conduction band of titania and further undesirable processes, including electron recombination at the titania-dye and titania-electrolyte interfaces. Additionally, we applied passivation of titania surface by the molecular-capping post-treatment (after dye sensitization). A comparison between the popular and well-known in literature dye belonging to the indoline class of chemical compounds (D149) with its alkoxysilyl derivative may be important from the point of view of future modified dye performance in DSSC systems [1].

Theoretical calculations provide that both for D149 and the modified dye (D149Si) the LUMO level is higher than the conduction band (CB) edge of titania resulting the thermodynamic driving force for the efficient electron injection from the excited state of dye to the CB of titania. Moreover, the HOMO of both dyes is mainly localized over the indoline and the LUMO on the rhodamine moiety. For D149 the LUMO is localized closer to the anchoring group (carboxyl) than for D149Si (trimethoxysilyl group links to the chromophore *via* the phenyl-amide moiety resulting only in small electron distribution around the anchoring group). It was found that the photovoltaic parameters and charge transfer dynamics studied by the femtosecond transient absorption and electrochemical impedance spectroscopy were similar for D149 and D149Si. More significant differences were observed upon substitution of iodide by the cobalt-based electrolyte. Additionally, desorption of the dyes with alkoksysilyl group from titania surface is more difficult than with carboxyl one. Procedure of molecular passivation of titania surface by the post-sensitization capping was checked [1].