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Molecular engineering of Ruthenium-diacetylide organometallic complexes towards efficient green dye for DSSC.

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Abstract

Three new dyes encompassing the organometallic [Ru(dppe)₂] (dppe = 1,2-bis(diphenylphosphino)ethane) fragment were designed and prepared for application in dye-sensitized solar cells. Introduction of the strong electron-withdrawing benzothiadiazole (BTD) unit as an additional acceptor in the attracting ligand led to original D-[M]-A-π-A' architectures. In particular the use of a thienyl-BTD motif led to a narrow bandgap sensitizer with deep-green coloration. The dye afforded 5.2 % power conversion efficiency in TiO₂-based DSSC device in the presence of the iodine/iodide couple as redox mediator. A joint experimental and theoretical study of the new dyes is reported.

Keywords

Dye-sensitized solar cells; Benzothiadiazole; Ruthenium-diacetylide complexes; DFT calculations; Organometallics; Photovoltaics.

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