

On the performance of ruthenium dyes in dye sensitized solar cells: A free cluster approach based on theoretical indexes

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© Springer-Verlag Berlin Heidelberg 2016. The performance of ruthenium dye sensitized solar cells (DSSC) with different types of ligand was studied by means of a theoretical model where the ruthenium complex is bound to two $[\text{Ti}(\text{OH})_3]^+$ units, instead of the more usual cluster TiO_2 model. Electron injection is proposed to proceed from a thermalized 3MLCT state rather than from higher vibrational excited states. The efficiency of the dye linked to the two $[\text{Ti}(\text{OH})_3]^+$ units was determined in terms of a global index (η), calculated as the product of three theoretical indexes (FI) built from the results of time-dependent density functional theory (TDDFT) calculations. The index considers the harvested and delivered energy (F1), the charge transferred to the semiconductor (F2), and dye regeneration (F3). The results show that this set of parameters is unique for each dye, and allows the comparative evaluation of the performance of a series of dyes, with a different ancillary ligand at each sta