

عنوان مقاله:

Ruthenium Sensitizer Functionalized by Carboxylic Anchoring Groups for Dye-Sensitized Solar Cells

محل انتشار:

چهارمین همایش ملی کاربرد فناوری های نوین در علوم مهندسی (سال: 1395)

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خلاصه مقاله:

Ru(II) dyes have been proposed for dye-sensitized solar cells (DSSC) as possible low-cost photovoltaic devices. Herein, a new synthesized Ru(II) dye labeled Ru (L2) (SCN)₂ is considered for solar cell applying. Using ab-initio density functional theory (DFT) with the B9LYP exchange-correlation functional, the electronic structure and also the visualized molecular orbital, including HOMO-5, HOMO, LUMO, and LUMO+5 was regarded. Our result showed that the HOMO is localized the Ru metal, while the LUMO is localized on the ancillary ligands and carboxylic groups. As the carboxylic groups are responsible for links to the TiO₂ surface, that molecular orbital categories provide the charge transfer from the LUMO states of the dye to the conduction band of TiO₂. This arrangement proposed the capability of the dye for solar cell applying. In addition the calculation band gap energy between HOMO and LUMO is 2.25 eV .enhancing the ability of sensitizer to photon absorption

کلمات کلیدی:

DSSC, Ru dye, HOMO, ancillary ligands

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