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Computational study of the effect of spin-orbit coupling on photo-physical properties of metal complex for dye sensitized solar cell

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Using transition metal complexes as dye sensitizer have attracted a lot of attention for researchers, especially in dye sensitized solar cell (DSCs). Ruthenium complex has been used for DSCs because they have many excellent photovoltaic properties. Unfortunately it has low metal-to-ligand charge transfer (MLCT) molar extinction coefficient (ε) in NIR region. Replacement ruthenium metal center $[Ru(bpy)3]^{2+}$ by osmium complex $[Os(bpy)3]^{2+}$, reported by Fantacci and colleagues in 2014, featuring the low energy absorption band in the NIR region. Osmium (II) complex have shown excellent photosensitization, broad absorption spectra in NIR region due to enhanced singlet-triplet charge-transfer transitions, suitable excited and ground state energy levels, good thermal and chemical stabilities, and shorter lifetimes of excited triplet metal-to-ligand charge transfer (^{3}MLCT). Our strategy of new sensitizer dyes is replacing ruthenium with osmium as metal center in complexes dyes, together with the modification of ligand by long alkyl chain. We present optical properties of the Os-3, CYC-33O, and CYC-33R complexes for dyes sensitized solar cells (DSCs), were calculated density functional theory (DFT) and time-dependent density functional theory (TDDFT) use B3LYP functional including non-relativistic (NR), scalar relativistic (SR) and spin-orbit coupling (SOC). They were shown that the effect of SOC on absorption spectra in near infra-red (NIR) region, produce low energy absorption band. It was demonstrated of Os-3 and CYC-33O arise triplet metal-to-ligand charge transfer (^{3}MLCT) state as spin-forbidden transitions above 700 nm. The metal ligand environment has effect to strength of SOC. The calculation results reveal that CYC-33O complex has strongest SOC in 770 nm and lowest energy band gap at 2.525 eV. While, CYC-33R complex provide higher excitation energy, produce weaker SOC. That is, CYC-33O complex may have improved light harvesting efficiency, which makes CYC-33O complex as a promising sensitizer for future DSCs applications.

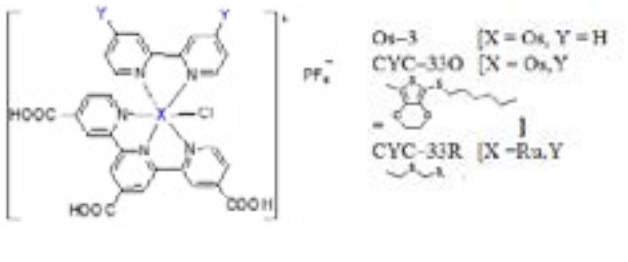

Figure 1: Molecular geometries of complexes dye in this study.

Biography

Ratna Juwita has her expertise in solar cells and passion in improving efficiency of dye sensitizer. She was an assistant in Biochemistry Laboratory and Inorganic Laboratory, Department of Chemistry, University of Brawijaya, Indonesia. She received scholarship on 2011-2013 from Ministry of National Education, Indonesia for her master degree at National Central University and University Brawijaya. Her master research is about the structural and dynamical properties of human serum albumin and its mutants by molecular dynamics simulations. After finishing her master degree, in 2014 she received scholarship for her doctoral degree in National Central University so far.

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