
Ruthenium (II) complexes with new large-surface ligands based on electron-accepting expanded pyridiniums: insights from Density Functional Theory

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Résumé

With the aim of designing new inorganic photosensitizers for photovoltaic applications, the structural and electronic properties of two Ru(II) complexes containing terpyridine-based ligands derived from expanded pyridinium - both branched-polyphenyl-and fused-polycyclic - were investigated by the means of Density Functional Theory (DFT) and Time-dependent DFT(TDDFT). In particular, the structure and electronic absorption of the fused architectures - including the isolated ligand and its complex - were compared to those of their respective branched precursors with the aim to account for the their enhanced electronic features in the visible spectral region. The theoretical insights gained from the "large-surface" ligand and its associated complex open the route for a joint experimental and theoretical design of new inorganic photosensitizers based on fused expanded pyridiniums.

Mots-Clés: inorganic photosensitizers, photovoltaic applications, Ru(II) complexes, terpyridine, based ligands, Time, dependent DFT(TDDFT).

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