

# Development of a new Ru(II) complex containing a donor-spacer-acceptor group for dye-sensitized solar cell (DSSC) applications

**Juliana da Silva Goulart (PG)\*, Fernando de Carvalho da Silva (PQ), Fabio da Silva Miranda (PQ)**

[julianagoulart@outlook.com](mailto:julianagoulart@outlook.com)

Institute of Chemistry, Universidade Federal Fluminense, Niterói, RJ, Brazil, 24020-140.

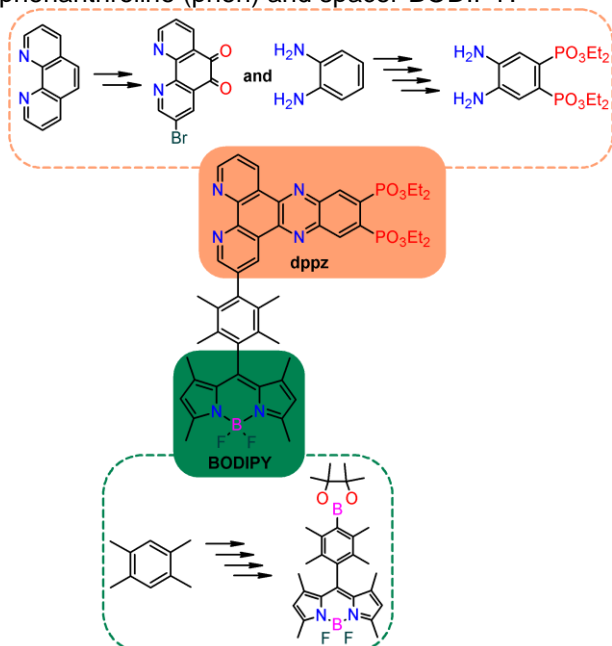
Keywords: photochemistry, donor-spacer-acceptor, BODIPY, ruthenium, DSSC, rational design.

## Introduction

Dye-sensitized solar cell (DSSC) has attracted great interest due to its low cost. In order to produce more efficient solar cells, new ligands and complexes containing donor-spacer-acceptor groups have been studied. This kind of ligand favors photo-induced charge separation and increases the absorption range in the visible region.<sup>1</sup> Ruthenium complexes have been studied as sensitizers due to their stable oxidation states and photochemical properties.<sup>2</sup> This work aims to develop a new ruthenium(II) complex with a rigid ligand (DTMBB-(PO<sub>3</sub>H<sub>2</sub>)<sub>2</sub>) that contains two different chromophores: dppz and BODIPY. The architecture contributes to generate a long-lived excited state besides avoiding non-radiative loss of energy, important factors to achieve an efficient solar cell.

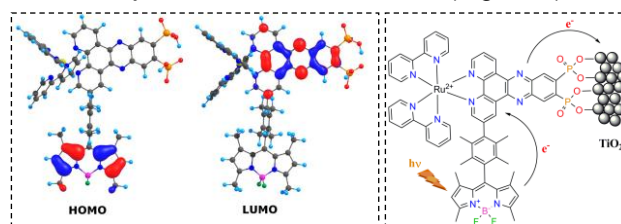
## Results and Discussion

The summarized synthetic route for the preparation of the ligand DTMBB-(PO<sub>3</sub>Et<sub>2</sub>)<sub>2</sub> is shown in Scheme 1. It was divided into three building blocks: diamine, phenanthroline (phen) and spacer-BODIPY.



**Scheme 1.** Synthetic route of the ligand DTMBB-(PO<sub>3</sub>Et<sub>2</sub>)<sub>2</sub> separated in building blocks.

The molecule was designed to transfer electrons under optical excitation from the donor (D) group (BODIPY) to the acceptor (A) group (dppz). The rigid spacer and the methyl groups in BODIPY core restrict rotation and provide the system an orthogonal arrangement. The major mechanism for the energy transfer between D and A is through-space, known as Förster mechanism. Due to the synthetic challenges and the desired features, preliminary DFT calculations were carried out in the TURBOMOLE 6.6 package (using PBE0/def2-SVP method) in order to prove the electron migration from BODIPY to dppz. The phosphonic acid group bonded in dppz unit will attach the complex on the semiconductor oxide surface (TiO<sub>2</sub>) and allow electron injection in its conduct band (Figure 1).



**Figure 1.** HOMO and LUMO orbitals of [Ru(bpy)<sub>2</sub>DTMBB-(PO<sub>3</sub>H)<sub>2</sub>] complex and a proposed mechanism for the photo-induced electron transfer from the complex to the TiO<sub>2</sub>.

The optimized geometry shows the orthogonality between the spacer and the chromophores. The theoretical calculations also showed that the HOMO and LUMO energy levels (-5.99 and -2.98 eV, respectively) match the conduction band edge of TiO<sub>2</sub> (around -4.0 eV),<sup>3</sup> which ensure an efficient electron injection.

## Conclusions

The theoretical results show that the complex has a great potential as sensitizer to DSSC devices.

## Acknowledgment

FAPERJ, CNPq, CAPES and PROPI-UFF.

<sup>1</sup>Fortage, J.; Puntoriero, F.; Tuyéras, F.; Dupeyre, G.; Arrigo, A.; Ciofini, I.; Lainé, P.; Campagna, S. *Inorg. Chem.* **2012**, 5342-5352

<sup>2</sup>Reynal, A.; Palomares, E. *Eur. J. Inorg. Chem.* **2011**, 4509-4526.

<sup>3</sup>Grätzel, M. *Nature* **2001**, 338-344.