High performance dye-sensitized solar cells using Ru(II) 4,7dicarbazole-1,10-phenanthroline based dye

Andressa V. Müller¹ (PG), Luiz Duarte Ramos¹ (PG), Karina Passalacqua Morelli Frin¹ (PQ), Kleber Thiago de Oliveira² (PQ), <u>André S. Polo¹ (PQ)</u>*.

¹Centro de Ciências Naturais e Humanas, Universidade Federal do ABC – UFABC, Av. dos Estados, 5001, 09210-580, Santo André – SP, Brazil. ²Departamento de Química, Universidade Federal de São Carlos – UFSCAR, Rodovia Washington Luis, km 235, 13565-905, São Carlos – SP, Brazil *andre.polo@ufabc.edu.br

Keywords: Dye-sensitized solar cells, energy conversion, Ru(II) tris-heteroleptic dyes, molecular engineering

Abstract

DSSCs synthesized by cis-[Ru(cbz₂-phen)(dcbH₂) (NCS)₂] achieved higher efficiency than cis-[Ru (dcbH₂)₂(NCS)₂], N3.

Introduction

Ruthenium(II) tris-heteroleptic compounds based on 1,10-phenanthroline have attracted attention for their use in dye-sensitized solar cells (DSSCs).1-3 The introduction of two aromatic groups on the 4 and 7 positions of 1,10-phenanthroline can increase the molar absorptivity of the sensitizer and directly result in higher photocurrent generation as well as in overall efficiency of the solar cell.³ In this context, carbazole is a potential substituent that already shown improvements on the stability and lightharvesting capacity of 2,2'-bipyridine based Ru(II) dyes.4 work, In this cis-[Ru(cbz₂phen)(dcbH₂)(NCS)₂], cbz₂-phen = 4,7-dicarbazole-1,10-phenantrholine and $dcbH_2 = 4,4'$ -dicarboxylic acid 2,2'-bipyridine was synthesized, characterized and employed as a dye-sensitizer for solar cells.

Results and Discussion

The compound exhibits broad and intense MLCT bands (ϵ_{525nm} = 1.8 x 10⁴ L mol⁻¹ cm⁻¹ and ϵ_{375nm} = 1.4 x 10^4 L mol⁻¹ cm⁻¹ in ethanol) that overlap the visible spectrum and is capable of sensitize TiO₂ films. The energy levels of cis-[Ru(cbz₂phen)(dcbH₂)(NCS)₂] are adequate for its use in DSSCs, exhibiting emission maxima at 790 nm, E_{1/2} = +1.07 V vs. NHE, E(S*/S⁺) = -0.79 V vs. NHE and $E_{0-0} = 1.86 \text{ eV}$. DSSCs sensitized by *cis*-[Ru(cbz₂phen)(dcbH₂) (NCS)₂] and cis-[Ru(dcbH₂)₂(NCS)₂], N3, were characterized by current-voltage curves, Figure 1. The higher V_{OC} and J_{SC} values than for N3 lead cis-[Ru(cbz₂-phen)(dcbH₂)(NCS)₂] to overcome the efficiency of N3, as well as other published ruthenium(II) *tris*-heteroleptic dves containing phenanthroline derivatives ligands.

Besides thermodynamic parameters, the π delocalized carbazole rings become more coplanar to phenanthroline rings in triplet excited state resulting in an increase on its lifetime, favoring the

39ª Reunião Anual da Sociedade Brasileira de Química: Criar e Empreender

electron injection from triplet excited state in addition to the hot injection from singlet one. $^{\rm 5}$



Figure 1. Current-voltage curves measured for solar cells sensitized by *cis*-[Ru(cbz₂-phen)(dcbH₂)(NCS)₂] (-) or N3 (-) under A.M. 1.5G irradiation ($P_{irr} = 100$ mW cm⁻²).

Conclusions

cis-[Ru(cbz₂-phen)(dcbH₂)(NCS)₂], was synthesized, characterized and applied as sensitizer in DSSCs. The high efficiency observed is ascribed to the carbazole groups, capable of change the energy levels of the dye resulting in thermodynamically favorable electron injection and dye regeneration processes. The electron injection from triplet state also enhances the performance of the solar cells.

Acknowledgements

FAPESP(2015/00605-5,2015/13149-8,2013/06532-4 and 2013/25173-5).

¹Carvalho, F.; Liandra-Salvador, E.; Bettanin, F.; Souza, J. S.; Homemde-Mello, P.; Polo, A. S. Inorg. Chim. Acta 2014, 414, 145.

²Müller, A. V.; Mendonça, P. S.; Parant, S.; Duchanois, T.; Gros, P. C.; Beley, M.; Polo, A. S. J. Braz. Chem. Soc. 2015, 26, 2224.

³ Sun, Y. L.; Onicha, A. C.; Myahkostupov, M.; Castellano, F. N. ACS Appl. Mat. Inter. 2010, 2, 2039.

⁴ Chen, C.-Y.; Pootrakulchote, N.; Hung, T.-H.; Tan, C.-J.; Tsai, H.-H.; Zakeeruddin, S. M.; Wu, C.-G.; Grätzel, M. J. Phys. Chem. C. 2011, 115, 20043.

⁵ Damrauer, N. H.; Boussie, T. R.; Devenney, M.; McCusker, J. K. J. Am. Chem. Soc. 1997, 119, 8253.