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High molar extinction coefficient heteroleptic Ru(II)-mixed ligand polypyridyl complexes containing anthracenyl and 2-methyl-2-butenoic acid functionalities: New emerging dyes for dye-sensitized solar cell application

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Dye-sensitized solar cells (DSSCs; Grätzel cells) are considered one of the promising solar cell technologies of the future. Traditionally, DSSCs utilize a mesoporous nanocrystalline TiO_2 film covered with ruthenium-bipyridyl-based dyes as the photoelectrode material and triiodide/iodide as the redox relay in the electrolyte. Such cells have reached conversion efficiencies above 11% at AM 1.5 solar irradiance. In the cells, the dye is one of the key components for high power conversion efficiencies. The pioneering studies using *cis*-dithiocyanatobis(4,4'-dicarboxylic acid-2,2'-bipyridine)-ruthenium(II) (N3) is a paradigm in this field. Major drawbacks of the N3 dye are low molar extinction coefficient, durability and lack of absorption in the red region of the visible spectrum. New focus and development in the dye-sensitized solar cell research comes from the preparation of amphiphilic heteroleptic N3-equivalents, nanocrystalline TiO_2 semiconductor, and/or electrolyte. It is on the basis of these major tasks of optimizing the conversion efficiencies of the DSSC that the current research work is undertaken.

This work describes the synthesis and characterization of new heteroleptic ruthenium(II) bipyridine/phenanthroline mixed ligand complexes bearing a simple anthracene anchored on unsaturated α,β-carboxylic acid functionality. The ruthenium complexes are constructed in a first step with the ligands bearing the required bromine functions, followed by a stepwise grafting of anthracene halide derivative promoted by palladium-carbide catalysis. The UV-vis absorption spectra of complexes in chloroform-methanol (1:1, v/v) solution displayed broad and low energy metal-to-ligand-charge transfer transitions (1MLCT) at λ_{max} between 520-700 nm (ε = 3.80-6.60 x 103 M^{-1} cm^{-1}) with a significantly enhanced band tail, improving red light absorptivity beyond 915 nm. At room temperature, complexes showed high intensity and appreciable emission wavelengths between 660 and 690 nm. The electrochemical redox properties of the complexes showed single- to multi- electronic transfer reactions. The solar to electrical energy conversion efficiency, DFT and EIS properties of the complexes are currently under investigation.

Biography

Adeloye Adewale Olufunsho received a B.Sc. (Hons.), Chemistry from the Ondo State University, Ado-Ekiti, Nigeria, 1994. He proceeded to study Pharmaceutical Chemistry at the Faculty of Pharmacy, Obafemi Awolowo University, Ile-Ife, Nigeria. He registered for a doctoral study at the University of Fort Hare, Alice, South Africa in 2008 and was awarded a Ph.D. in Chemistry in 2011. He has 17 published articles in peer-reviewed accredited journals to his credit with an appreciable number of citation volumes. He has worked as a postdoctoral research fellow at two different universities in South Africa.

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