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Optical sensitization of TiO_2 with modified Alq3 complexes

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Abstract – The optical sensitization and interfacial electron transfer dynamics between the Alq3 complex, tris(8-hydroxyquinoline)Aluminum(III), and anatase-titanium dioxide (TiO_2) semiconductor is investigated by atomistic time-dependent quantum mechanical methods. The Alq3 complex is a prototypical compound for OLED fabrication, however, despite the great success achieved with electroluminescent devices the compound has not been employed as the active optical material in photovoltaic cells. The work proposes a method for optical sensitization of TiO_2 with Alq3. The reported results are expected to motivate experimental work toward the realization of Alq3 based DSSC that incorporate the knowledge gained from Alq3-OLED technology, particularly regarding efficient mechanisms for carrier transport in solid-state dye sensitized solar cells (DSSC). In addition to its technological relevance, the system offers a rich framework for fundamental investigations of photoconversion mechanisms.

The optical sensitization of titanium dioxide (TiO_2) by covalent attachment of tris(8-hydroxyquinoline)aluminum(III) derivatives and the subsequent interfacial electron-hole pair separation are investigated by atomistic time-dependent quantum mechanical methods. Thin films of Alq3 are widely used as the optical medium in stable and high efficiency organic electroluminescent devices [1], but have not been used as the active optical compound in photovoltaic solar cells. In this study we propose a method of combining Alq3 derivatives with the catechol molecule to produce a stable molecular photosensitizer that absorbs in the visible and transfers the photoexcited electron into the TiO_2 semiconductor within the femtosecond time scale, for possible applications in dye sensitized solar cells (DSSC) [2].

A combination of theoretical methods is used to describe the sensitization process in the Alq3-catechol/TiO_2 system (Figure 1), including DFT based and CIS calculations for both molecular and extended systems as well as time-dependent quantum dynamics calculations [3,4].

The present study demonstrates that derivatized Alq3 complexes can be combined with catechol to produce a stable photosensitizer that binds strongly to the surface of anatase-TiO_2 and photosensitizes the semiconductor in the visible region. Ultrafast electron injection (within the fs time scale) from the unoccupied states of the Alq3-dye into the TiO_2 semiconductor is obtained. A new derivatization process with oligothiophenes is proposed to provide an efficient mechanism for electron-hole separation and dye regeneration (Figure 2).

The reported results are expected to motivate the development of inexpensive Alq3 based dye sensitized solar cells, building upon existing technology gained from the fabrication of solid-state Alq3 luminescent devices.

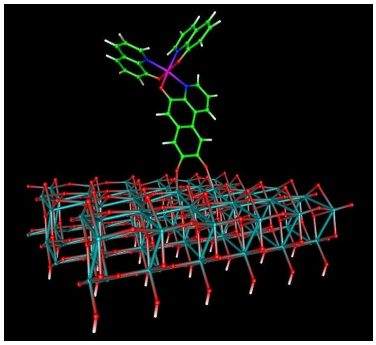

Figure 1: Alq3-catechol dye adsorbed on anatase-TiO_2.

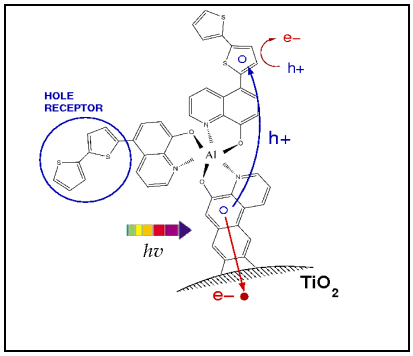

Figure 2: electron-hole pair separation and dye regeneration by redox mediator.

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