Theoretical Chemistry Colloquium

March 6, 2014 (Thu), 16:00-17:00

RCMS, 2nd floor, Chemistry Gallery

Quantum Chemical Studies of organic sensitizers with modified donor units for efficient dye-sensitized solar cells

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Abstract: *Electronic structures and absorption spectra of a new series of organic donor-π-acceptor dyes used for dye sensitized solar cells (DSSCs) with modified amine moieties as donor groups including thiophene and fluorene-connected carbazole on top of thiophene, and π-spacer with thiophene (1 to 3 units) were molecularly designed and theoretically investigated by density functional theory (DFT) and time-dependent DFT (TDDFT). The nature of intramolecular charge transfer (ICT) of all dyes was elucidated by means of frontier molecular orbital analysis. The prototype of DSSCs performance was simulated using the chemisorption of dyes onto the $(TiO_2)_{38}$ cluster and the nature of the electron injection mechanism was identified. The efficient prediction of dyes in terms of the light-harvesting efficiency (LHE) at the maximum absorption wavelength (λ_{max}) and the driving force ΔG_{inject} of the electron injection from the excited state of dyes to the conduction band (CB) of TiO2 was carried out and discussed. The presented work is expected to assist in the molecular design of new metal-free organic dyes for use in DSSCs yielding highly efficient performance.*

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