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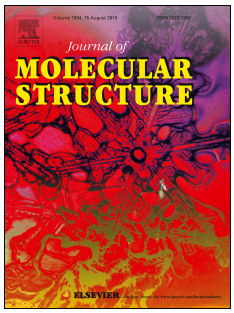

DFT and TD-DFT calculations of metallotetraphenylporphyrin and metallotetraphenylporphyrin fullerene complexes as potential dye sensitizers for solar cells

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DFT and TD-DFT calculations of metallotetraphenylporphyrin and metallotetraphenylporphyrin fullerene complexes as potential dye sensitizers for solar cells

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Abstract

Density functional theory (DFT) and time-dependent DFT calculations have been employed to model metallotetraphenylporphyrin dyes and metallotetraphenylporphyrin –fullerene complexes in order to investigate the geometries, electronic structures, the density of states, non-linear optical properties (NLO), IR–vis spectra, molecular electrostatic potential contours, and electrophilicity. To calculate the excited states of the tetraphenyl porphyrin analogues, time-dependent density functional theory (TD-DFT) are used. Their UV-vis spectra were also obtained and a comparison with available experimental and theoretical results is included. The results reveal that the metal and the tertiary butyl groups of the dyes are electron donors, and the tetraphenylporphyrin rings are electron acceptors. The HOMOs of the dyes fall within the $(TiO_2)_{60}$ and $Ti_{38}O_{76}$ band gaps and support the issue of typical interfacial electron transfer reaction. The resulting potential drop of Mn-TPP-C_{60} increased by ca. 3.50 **%** under the effect of the tertiary butyl groups. The increase in the potential drop indicates that the tertiary butyl complexes could be a better choice for the strong operation of the molecular rectifiers. The introduction of metal atom and tertiary butyl groups to the tetraphenyl porphyrin moiety leads to a stronger response to the external electric field and induces higher photo-to-current conversion efficiency. This also shifts the absorption in the dyes and makes them potential candidates for harvesting light in the entire visible and near IR region for photovoltaic applications.

Keywords: tetraphenylporphyrin ; fullerene; dye sensitizers; solar cells; dFT calculations

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