Improvement of photovoltaic performance by substituent effect of donor and acceptor structure of TPA-based dye-sensitized solar cells

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We report a computational study of a series of organic dyes built with triphenylamine (TPA) as an electron donor group. We designed a set of six dyes called (TPA-n, where n = 0?5). In order to enhance the electron-injection process, the electron-donor effect of some specific substituent was studied. Thus, we gave insights into the rational design of organic TPA-based chromophores for use in dye-sensitized solar cells (DSSCs). In addition, we report the HOMO, LUMO, the calculated excited state oxidized potential Edye*(eV) and the free energy change for electron-injection ?Ginject(eV), and the UV-visible absorption bands for TPA-n dyes by a time-dependent density functional theory (TDDFT) procedure at the B3LYP and CAM-B3LYP levels with solvent effect. The results demonstrate that the introduction of the electron-acceptor groups produces an intramolecular charge transfer showing a shift of the absorption wavelengths of TPA-n under studies. [Figure not available: see fulltext.]

Density functional theory

Electronic absorption spectra

Molecular design

Organic dye-sensitized solar cells

aniline

triphenylamine

unclassified drug

coloring agent

terphenyl derivative

absorption

Article

chromatophore

density functional theory

donor

dye sensitized solar cell

electrical equipment

electron

priority journal

semiconductor

ultraviolet radiation

chemistry

solar energy

Coloring Agents

Solar Energy

Terphenyl Compounds