

2020-01-01

# Tuning optoelectronic properties of triphenylamine based dyes through variation of pi-conjugated units and anchoring groups: A DFT/TD-DFT investigation.

Deoqratias, Geradius

Elsevier Inc.

---

<https://doi.org/10.1016/j.jmgm.2019.107480>

*Provided with love from The Nelson Mandela African Institution of Science and Technology*

# Tuning optoelectronic properties of diphenylamine based dyes through variation of pi-conjugated units and anchoring groups: A DFT/TD-DFT investigation

Geradius Deogratias, Nicola Serianic, Tatian Pogrebnaya, Alexander Pogrebnoi

To download full text click that link

DOI:

<https://doi.org/10.1016/j.jmglm.2019.107480>

Abstract

Dye-sensitized solar cells (DSSCs) have attracted widespread attention due to their unique features. In the present work, molecular engineered triphenylamine based dyes featuring donor-bridge-acceptor architecture have been considered and investigated for suitable properties for DSSCs applications. Hydantoin anchoring group has been introduced replacing the commonly used cyanoacrylic acid to improve the long-term stability of the device. Results on the effects of varied anchoring groups and pi-spacers have been interpreted from the viewpoint of DFT/TD-DFT calculations. Designed sensitizers exhibit suitable light-harvesting efficiencies, excited-state lifetimes, electron injection and regeneration abilities. Red-shifted electronic spectra are observed for three hydantoin dyes compared to others in the same family. Further analysis of chemical descriptors and observation from full-electron donor-acceptor map reveal that the three dyes among nine are potential materials with promising properties towards improving DSSCs performance.

**Keywords**

**Cyanoacrylic; DSSC; Hydantoin; Optoelectronics; Triphenylamine**