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A theoretical investigation of decorated novel triazoles as organic dyes in dye sensitized solar cells

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This research presents DFT and TD-DFT calculations for eight 1,2,4-triazole compounds (A1-A8) that were theoretically evaluated as organic dyes in dye sensitized solar cells (DSSCs). The parameters used in this evaluation included, oscillator strengths, electron diffusion constants, electron injection efficiencies, electron collection efficiencies, highest occupied molecular orbitals (HOMO), lowest unoccupied molecular orbitals (LUMO), amongst others. These parameters play a significant role in determining the efficiency of the dye as rapidly diffusing electrons will be more readily available for electron injection into the conduction band of the semi-conductor where they can participate in the current flow and be regenerated back into the dye via an electrolyte provided that the HOMO of this electrolyte lies at a higher energy level than the HOMO of the dye. Moreover, the LUMO of the dye should also lie at a higher energy level than the LUMO of the conduction band of the semi-conductor. More rapid diffusion can be facilitated by conjugated systems that consists of donor, linker (π-spacer) and acceptor fragments where electrons are localized across the donor and being delocalized towards the acceptor via the linker. In this study, starburst and alkoxy phenyl groups acted as the donors, while the 1,2,4-triazole groups acted as the linker, and cyano acrylic acid acted as the acceptor group. Since the acceptor group must adhere to the semi-conductor for efficient electron injection, it is important that as much electrons as possible reaches this group. From this study, it was discovered that A2 was the most efficient organic dye.

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