# Solvent effect on the efficiency of triphenylamine-based dye-sensitized solar cells, molecular approach

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## Abstract

In this research, dynamics, and kinetics of some metal-free organic dyes based on triphenylamine having a D-π-A type structure were investigated in the gas phase and solvent (ethanol, dichloromethane, toluene, tetrahydrofuran, chloroform, and dimethylformamide) using the quantum chemistry calculations. These structures consist of triphenylamine as the donor linked to the acceptor units of cyanoacrylic acid and benzoic acid via different π-conjugated systems. The obtained results show that TC601 dye having the ethynyl anthracene phenyl ?-conjugated system has the preferred charge/hole transfer properties (?Ginj/?Greg), which in ethanol as the solvent, the lowest values of ?Ginj and ?Greg were evaluated. Molecular spectroscopic properties of the studied dyes reveal that H-P and F-P dyes have favorable molar absorption coefficients in all media. Also, the behaviors of the light-harvesting efficiency (LHE) and incident photon to current efficiency (IPCE) as the functions of the wavelength were analyzed, which show that the presence of solvent increases the values of IPCE and LHE for most studied dyes in comparison with the gas phase. Finally, based on different analyses, TC601 as the dye and ethanol as the solvent are proposed as the preferred candidates to be applied in the DSSCs.

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