Effect of Inserting Azabenzenes Linkers into TPABased Dye Sensitizers for Use in Solar Cells: DFT and TDDFT Calculations

AHMED M EL-NAHAS1, RAMY E FARAG1, MORAD M EL-HENDAWY, SAFINAZ H EL-DEMERDASH and SHABAN Y SHABAN

Abstract:

Abstract: Density functional theory (DFT) and time-dependent density functional theory (TDDFT) were used to study optical and electrochemical properties of a new series of dye sensitizers for use in dye-sensitized solar cells (DSSCs). The dyes include triphenylamine(TPA) unit as an electron donor and cyanoacrylic acid moiety as an electron acceptor/anchoring groups with different -linkers. The effect of linkers on the performance of these dyes as photo-sensitizers was investigated. The linkers are benzene and azabenzenes and their hydrocarbon parent systems. The results indicated that the highest occupied molecular orbital (HOMO) is delocalized over the TPA unit and - linker while lowest unoccupied molecular orbital (LUMO) is localized on the electron acceptor and -linker. The HOMO level of the investigated dyes is located below the HOMO level of the I-/I3 - redox couple while the LUMO is situated above the conduction band of TiO2. The gradual insertion of nitrogen at benzene bridge decreases HOMOLUMO energy gap. This ensures good electron injection and dye regeneration. They also introduce gradual red shift by increasing nitrogens at benzene bridge which is an indicator for enhancing photocurrent. The results suggest the possibility of design of efficient photovoltaic organic materials in DSSCs from the selected dyes.

Keywords:

DSSCs, Triphenylamine(TPA), Azabenzenes, TD-DFT, -linkers, FMO

Published In:

Chemical Science Transactions , 5(2) , 399-409.