**ABSTRACT**

Incorporation of tetradecyloxy and carboxamide groups in trans-stilbene molecule (dye) has been investigated first time for Dye Sensitized Solar Cells (DSSCs) applications. To understand the changes in electronic structure, geometry, dipole moment and polarizability of the mentioned dye architecture has been carried out by using density functional theory (DFT) and time dependent DFT calculations using hybrid functional B3LYP method. Further, the semiconductor TiO2 is also used as a model to evaluate the photo conversion efficiency of the chosen dye architecture. Results reveal that tetradecyloxy and carboxamide groups act as an excellent donor and acceptor groups respectively which give rise to larger difference in excited state dipole moment than the ground state. This kind of stilbene based metal free organic dyes are act as a promising sensitizer for practical DSSCs applications.