**ABSTRACT**

Stilbene based metal free organic dye sensitizer has been designed first time for dye sensitized solar cells applications. The geometries, electronic structures and dipole moment of the chosen 4-amino-4′-dodecyloxy-stilbene dye sensitizer has been analyzed by using Density Functional Theory (DFT) and Time Dependent DFT (TD-DFT) calculations (based on hybrid functional B3LYP). The HOMO and LUMO energies of the dye 4-amino-4′-dodecyloxy-stilbene are −4.95 and −0.87 eV respectively calculated by using TD-DFT. To understand the conversion efficiency of the chosen dye architecture unit we selected TiO2 as a model for semiconductor. The values of polarizability and hyperpolarizability are 165. 94 and 347.74 a.u respectively based on DFT calculations. Results reveal that the selected dye sensitizer exhibits large dipole moment difference between the ground and excited state which is comparable to that of metal based dye sensitizers. Further the large dipole moment would be expected to give high photo-current conversion efficiency in practical DSSCs and also it is a promising candidate as a sensitizer for DSSC applications.