**ABSTRACT**

The metal-free organic dye sensitizer 2,3′-diamino-4,4′-stilbenedicarboxylic acid has been investigated for the first time for dye-sensitized solar cell applications. Density functional theory (DFT) and time-dependent DFT (TD-DFT) calculations (performed using the hybrid functional B3LYP) were carried out to analyze the geometry, electronic structure, polarizability, and hyperpolarizability of 2,3′-diamino-4,4′-stilbenedicarboxylic acid used as a dye sensitizer. A TiO2 cluster was used as a model semiconductor when attempting to determine the conversion efficiency of the selected dye sensitizer. Our TD-DFT calculations demonstrated that the twenty lowest-energy excited states of 2,3′-diamino-4,4′-stilbenedicarboxylic acid are due to photoinduced electron-transfer processes. Moreover, interfacial electron transfer between a TiO2 semiconductor electrode and the dye sensitizer occurs through electron injection from the excited dye to the semiconductor’s conduction band. Results reveal that metal-free 2,3′-diamino-4,4′-stilbenedicarboxylic acid is a simple and efficient sensitizer for dye-sensitized solar cell applications.