Abstract: In order to bridge the electronic structure information and photo-to-electric efficiency in dye-sensitized solar cells (DSSCs), a comprehensive understanding of sensitizers, their aggregation complexes, and hybrid sensitizers-semiconductor is a compelling need. The proposed proposal is focusing on structural calculations of excited state of sensitizers, simulations of optical spectra in solution, the photo-induced electron transfer from sensitizer to semiconductor cluster (such as Titania), and the adsorption/aggregation model on the surface of semiconductor. These theoretical calculations can help us to find the relation between the electronic details and photo-to-electric efficiency of sensitizers, further improve the performance of DSSCs.