Chapter 7
Concluding Remarks

In conclusion, after a brief introduction of the principles of Dye Sensitized Solar Cells (DSSCs), including their major components, the fabrication procedures and theoretical methodologies are discussed. These studies try to focus on the atomic mechanisms of dye adsorption and electron transport in DSSCs as obtained from accurate measurements through quantum chemical calculation. The electron injection rate and recombination rate are strongly influenced by various factors such as Donor, Spacer and Acceptor; more importantly the time scale for electron injection rate can be tuned by changing the efficiency of solar cell parameters namely short circuit current density \(J_{SC}\) and open circuit voltage \(V_{OC}\).

Based on the knowledge about the interface electronic structure and dynamics at the molecular level, the new dye molecules designed and state-of-the-art first principles calculations were carried out. Results show that upon systematic modifications on the existing dye structures, the optical absorption and energy levels could be gradually tuned. Stilbene and Triphenylamine based molecules have high dipole moment \(\mu\), polarizability \(\alpha_0\), first order hyperpolarizability \(\beta\) and second order hyperpolarizability \(\gamma\). Besides, Stilbene and Triphenylamine based molecules have good Non-linear optical property and DSSCs application.

In particular, D-\(\pi\)-A architecture by inserting Phenothiazine as donor based sensitizers could be promising candidates for enhanced red to infrared light absorption. This study opens a way for material design of new dyes with target properties to advance the performance of sensitizer in DSSCs.