Molecular Design, Synthesis and Performance Evaluation of Phenothiazine-based Small Molecules for Organic Solar Cells

Srikanth Revoju

Akademisk avhandling

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Fakultetsopponent: Docent Haining Tian
Institutionen för kemi – Ångströmslaboratoriet, Uppsala universitet, Sverige.

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Author
Srikanth Revoju

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Abstract
Photovoltaics offers one of the most promising routes to generate electricity in a clean way. As an emerging technology in photovoltaics, organic solar cells (OSC) have attracted a great deal of attention owing to their potential low-cost, lightweight, flexibility and solution processability. Although power conversion efficiencies above 12% have been achieved at this date, there is a great interest for new ideal materials to further improve the PCEs and address device durability, which are major concerns for the commercialization of this technology. The main objective of this thesis is to design and synthesize phenothiazine-based conjugate small molecules and explore their use as electron donor components in OSCs. Phenothiazine is a non-planar moiety with unusual "butterfly" type of geometry, which is known to reduce molecular aggregation and intermolecular excimer formation.

In the first study of this thesis, a small molecule based on a cyano-arylenevinylene building block with deep HOMO level was prepared. Although a high open-circuit voltage of 1.0 V was achieved, the tendency of the small molecule to crystallize in the active layer at a higher temperature and with time hindered the attainment of an optimal phase morphology required for the achievement of a higher efficiency. In the second and third studies, phenothiazine was used as a π-system bridge and as a core unit to construct small molecules based on symmetric and asymmetric frameworks with varying terminal electron-withdrawing groups. The electron-withdrawing property of the terminal units was found to have a significant influence on the optical absorption properties, electronic energy levels, molecular ordering, charge carrier mobility and morphology of the resulting active layers. In the fourth study, side-chain modification of the phenothiazine unit of symmetrically configured small molecules with an oxygen-containing (methoxyethoxy ethyl) side chain resulted in the enhancement of the dielectric constant. Although absorption properties were unchanged in solution, a dense π-π stacking was observed in the solid state.

In summary, it is demonstrated that phenothiazine is a promising candidate and worth exploring donor material for OSCs. Its versatility as a π-linker and as a central core unit in symmetric and asymmetric configurations has been explored. The use of nonplanar building blocks such as phenothiazine for the construction of donor materials is an interesting strategy for controlling molecular aggregation and difficult solution processability of small molecules if it is combined with a judiciously designed conjugate backbone.

Keywords
Organic solar cell, small molecule donors, phenothiazine, power conversion efficiency

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