Theoretical Model to Enhance the Hole mobility in Polymer based LED devices

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INTRODUCTION

PEDOT PSS - TD-DFT-B3LYP-D3-6-311G**

Theoretical Analysis

To Tune the Hole Mobility of PEDOT PSS

- Calculate oxidation potential, reduction potential, reorganization energies and carrier mobility
- Investigate the difference in hydrogen bonding in PEDOT-Water, PSS-Water, PEDOT - Water, PSS - Water/ PEDOT-DMSO, PSS-DMSO, PEDOT - DMSO, PSS - DMSO
- To study the separation of PSS chains from PEDOT in presence of DMSO by Molecular Dynamics (MD) simulations

Methodology

MOLECULAR DYNAMICS (MD) ANALYSIS

OUTCOME

- PSS-H and PSS-DMSO form strong hydrogen bonds with DMSO than water which is evident from intra and inter molecular hydrogen bonding distance
- Due to strong intermolecular hydrogen bonding of PSS-DMSO, the PSS chain moves apart from PEDOT chain, which is evidenced by MD simulation
- It is found that carrier mobility in PEDOT PSS increased from 1.09 x 10⁻⁶ cm²V⁻¹s⁻¹ to 4.03 x 10⁻⁶ cm²V⁻¹s⁻¹ in presence of DMSO

REFERENCES


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