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

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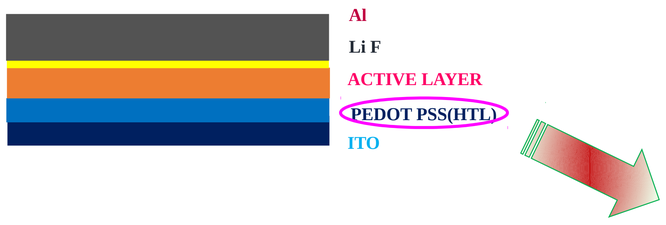
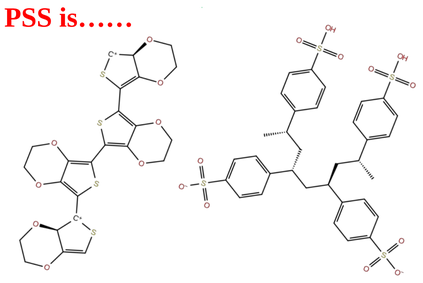
INTRODUCTION

- Poly(3, 4 – ethylenedioxythiophene)-Polystyrene sulphonate (PEDOT PSS) is widely used as hole transport layer (HTL) in Polymer based LED devices



Weight Percentage Composition of PEDOT PSS is……

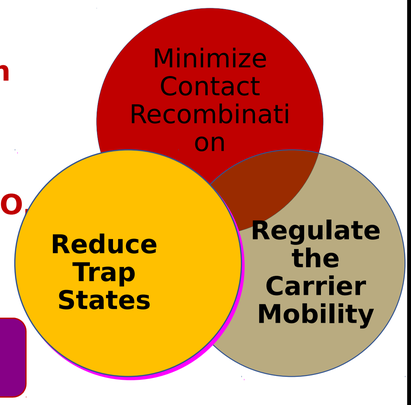
1:1.8



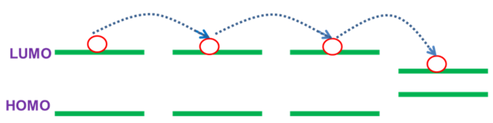
OBJECTIVES

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) simulation and its effect on carrier mobility**



CHARGE TRANSPORT



$$W_{ij} = \frac{J^2}{\hbar}\sqrt{\frac{\pi}{2Epk_BT}}\exp\left(-\frac{E_p}{2k_BT}\right)\exp\left(\frac{E_i - E_j}{2k_BT}\right)$$ Marcus Theory

$$W_{ij} = \vartheta_0 \exp\left(-\frac{2rij}{b}\right)\exp\left(-\frac{|E_i - E_i| + E_i - E_j}{2\,k_BT}\right)$$ Miller - Abraham Theory

$$\mu(T,F) = \mu_o exp\left[-\left(\frac{2\sigma}{3\,k_BT}\right)^2\right]\exp\left[c_o\sqrt{F}\left(\left(\frac{\sigma}{k_BT}\right)^2 - \Sigma^2\right)\right]$$

METHODOLOG

DFT and TD-DFT Calculation

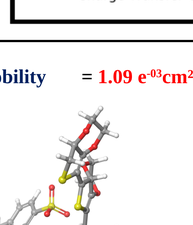
Optoelectronic Calculation

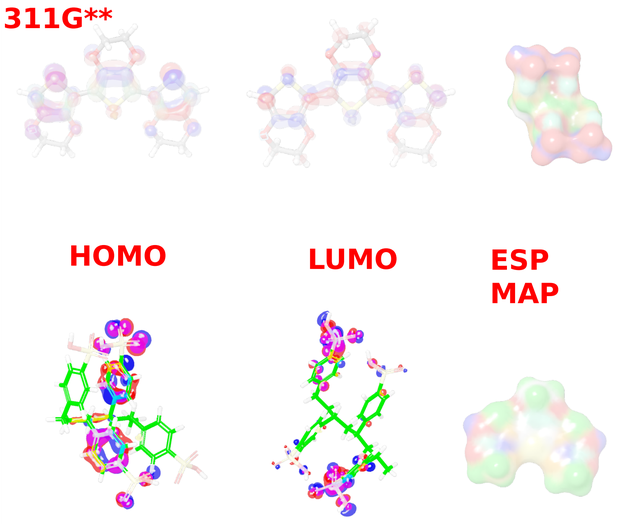
MD Simulation

→ **Hole Mobility Tuning of PEDOT PSS**

THEORETICAL ANALYSIS

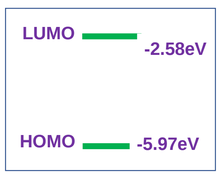
PEDOT PSS - TD-DFT-B3LYP-D3- 6-311G**





HOMO LUMO ESP MAP

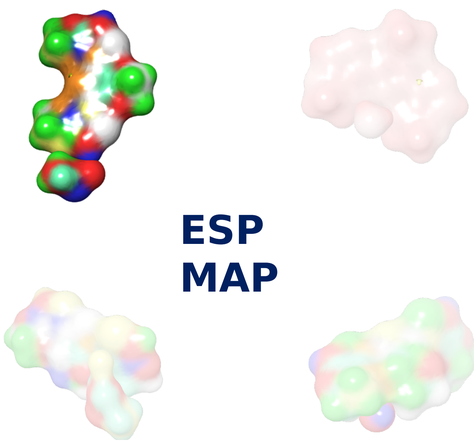
Hole Mobility = 1.09 $e^{-03}cm^2V^{-1}s^{-1}$



ENTRY ID	OP(eV)	RP(eV)	λ_h(eV)	λ_e(eV)	D
EDOT+ SS-	1.5	-1.94	0.895	0.811	15.76

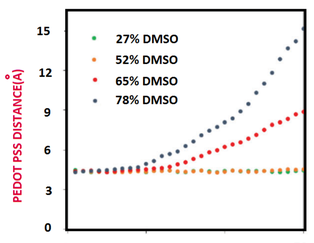
ENTRY	O_p(eV)	R_p (eV)	λ_h(eV)	λ_e(eV)	D
EDOT 2	1.88568	-2.2951	0.43242	0.46660	0.09
EDOT 3	1.19664	-2.02791	0.37390	0.3861	2.3
EDOT 8	0.01897	-1.68219	0.27119	0.25115	0.2

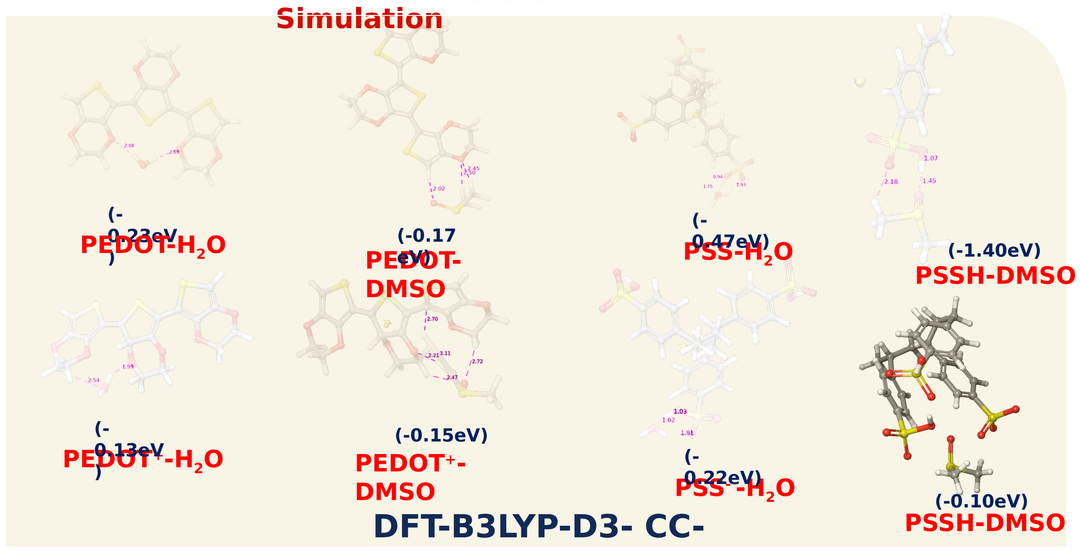
PEDOT-DMSO PEDOT-H_2O



ESP MAP

PEDOT+-DMSO PEDOT+-H_2O



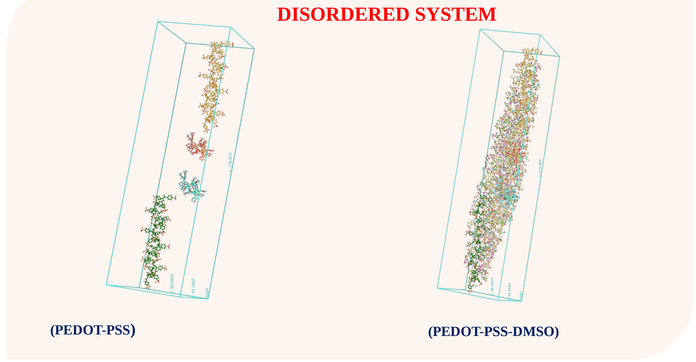


DFT-B3LYP-D3- CC-PVTZ

MOLECULAR DYNAMICS (MD) ANALYSIS

48-(16 C^+) EDOT Monomer

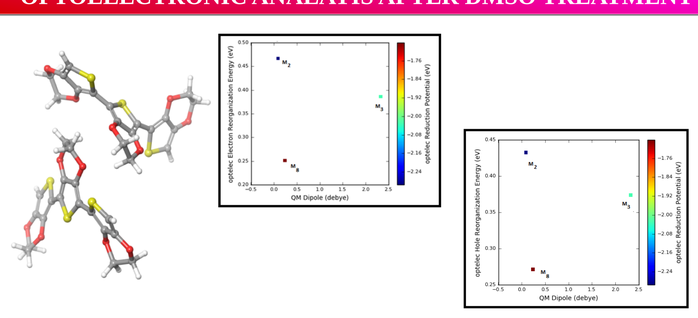
36-(6 O^-) SS Monomer



PEDOT CHAIN GET SEPARATED FROM PSS CHAINS

RESULTS: MD Analysis

OPTOELECTRONIC ANALAYIS AFTER DMSO TREATMENT



Direction	Charge Transfer coupling	Hopping rate	Mobility
Forward Transfer	0.065	25682.453	6.40 x $cm^2V^{-1}s^{-1}$
Reverse Transfer	9.61 x 10^{-4}	16895.45 x 10^5	

OUTCOME

- **PSSH and PSS^- 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 $e^{-03}cm^2V^{-1}s^{-1}$ to 6.40 x $cm^2V^{-1}s^{-1}$ in presence of DMSO**

FUTURE DIRECTIONS

- **Investigate the effect of interaction of medium of the HTL and the emissive layer during fabrication of the device**

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- Izarra, A. De; Park, S.; Lee, J.; Lansac, Y.; Jang, Y. H. Ionic Liquid Designed for PEDOT : PSS Conductivity Enhancement Ionic Liquid Designed for PEDOT : PSS Conductivity Enhancement. J. Am. Chem. Soc.2018

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