Structure Property relationships in Polymer solar cells Materials

Sandile Mamba

University of Kwazulau Natal (PMB)

4/12/2017

Table of Contents

Definition and Motivation

Definition

- Polymer based
- uses organic electronics

Motivation

◇ Dependence on non renewable energy sources

- Limited supply
- Non environmental friendly

◇ Solar energy is one alternative

- $\sim$ 6000 times the worldwide energy usage
- considered renewable

◇ Two types of solar cells

- Silicon
- Organic polymers

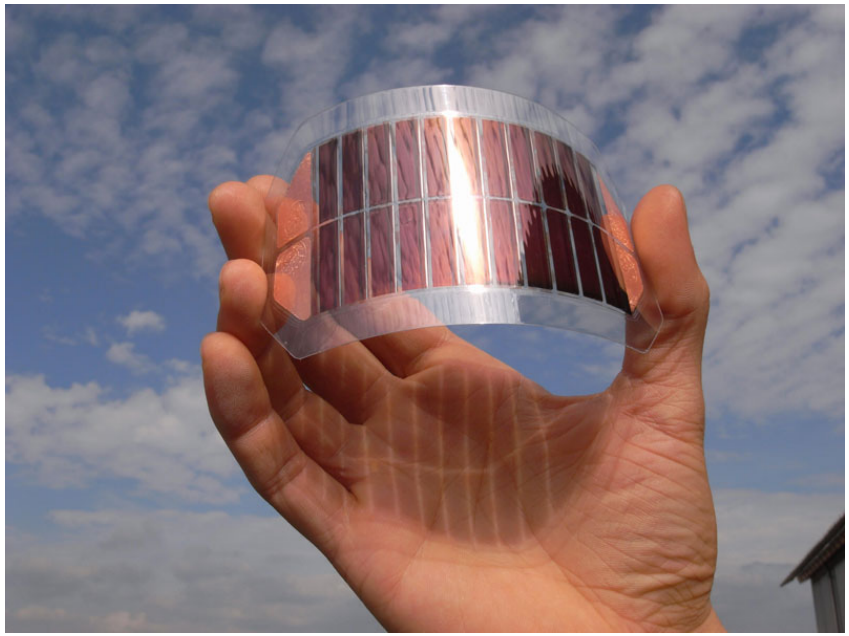
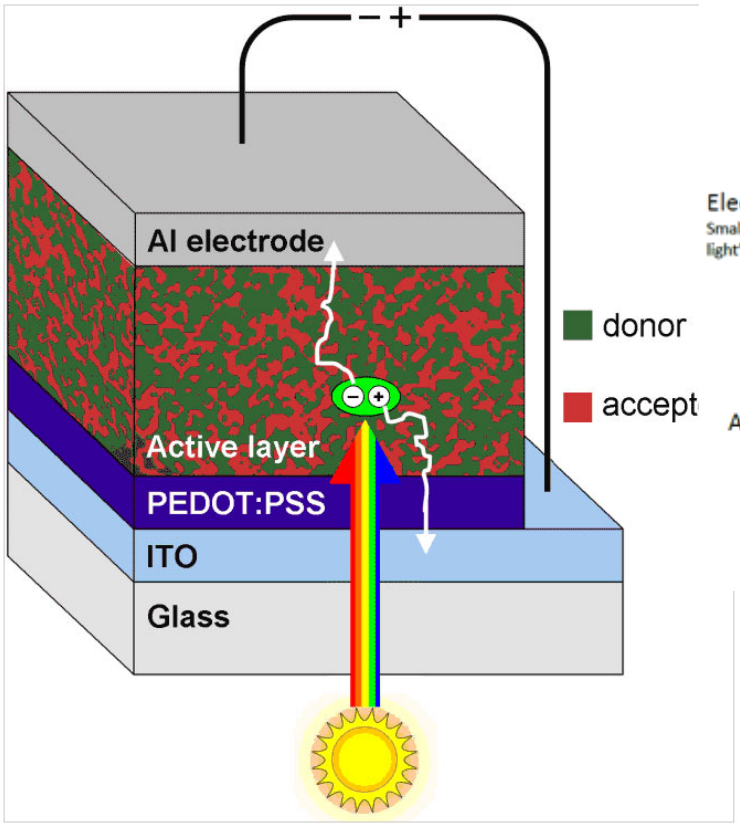
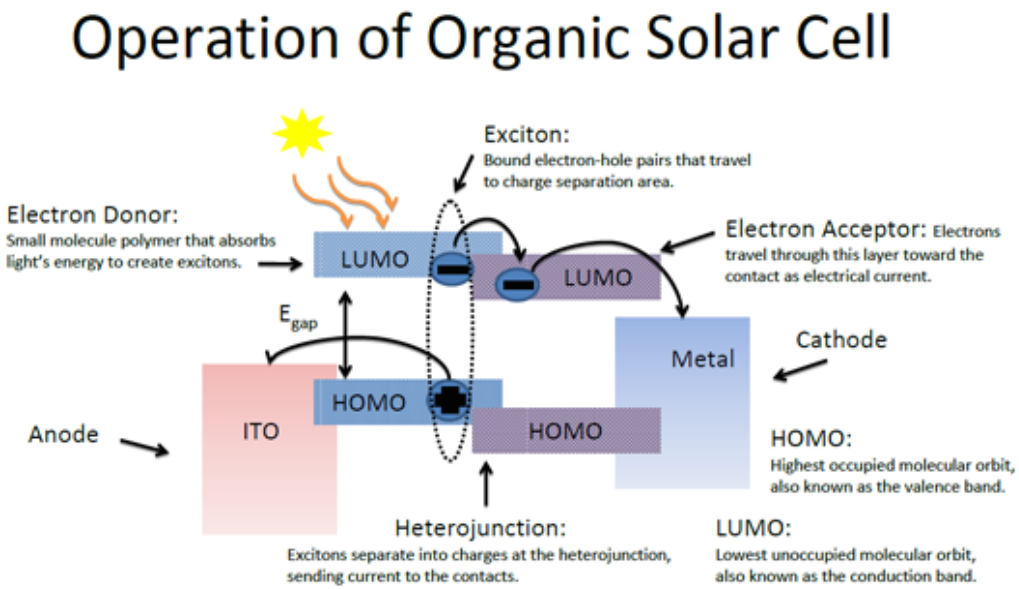


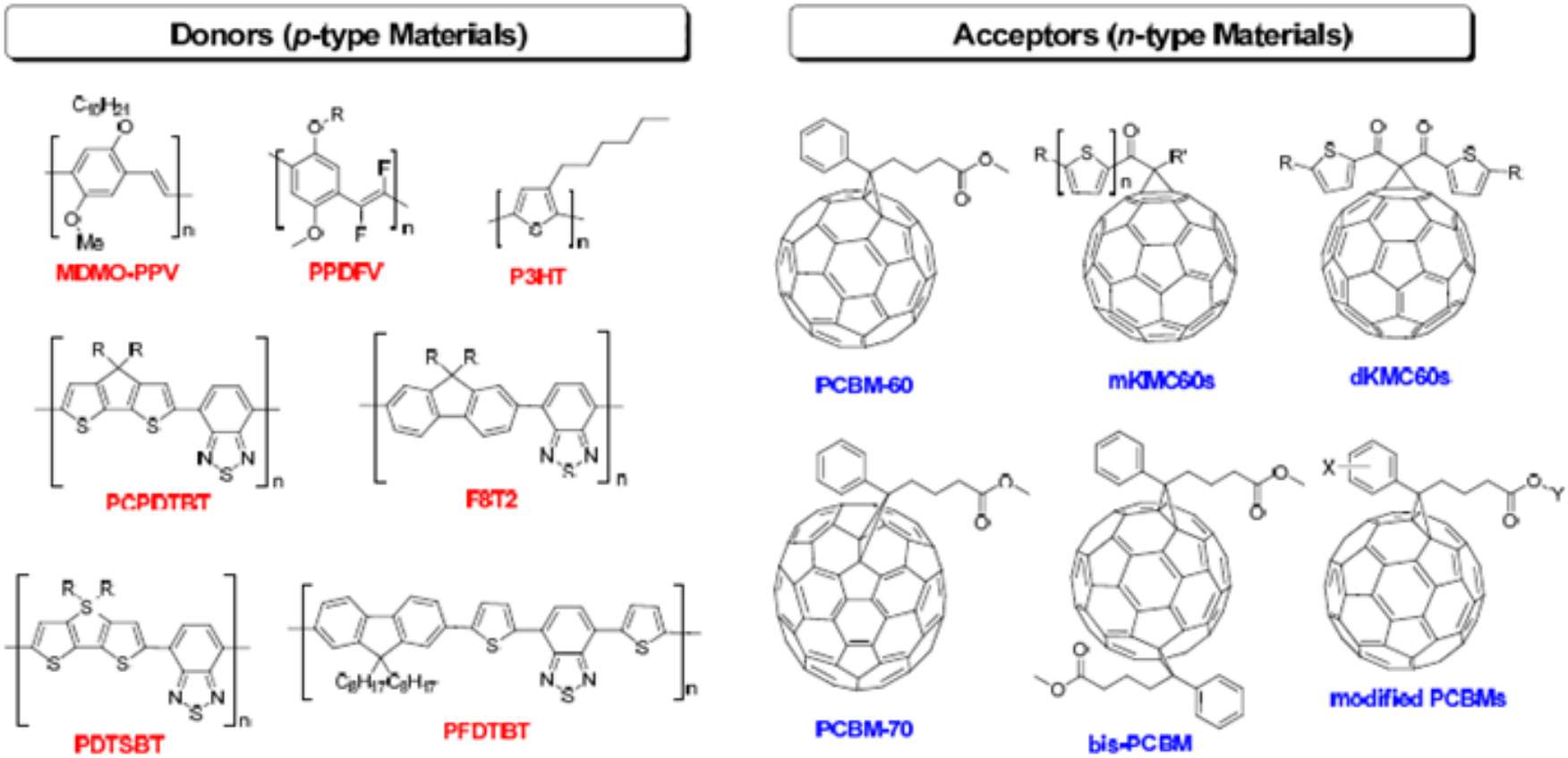
Figure: 1, showing a flexible organic solar cell

Overview of Organic Solar cells





Some donor and acceptor materials



Some requirements for organic solar cells

- HOMO should be $<$ -5.3 eV

J.F Laprade et al, 2010

- Lower bound of 1.3 eV for band gap

J.F Laprade et al, 2010

- Plenary side chains

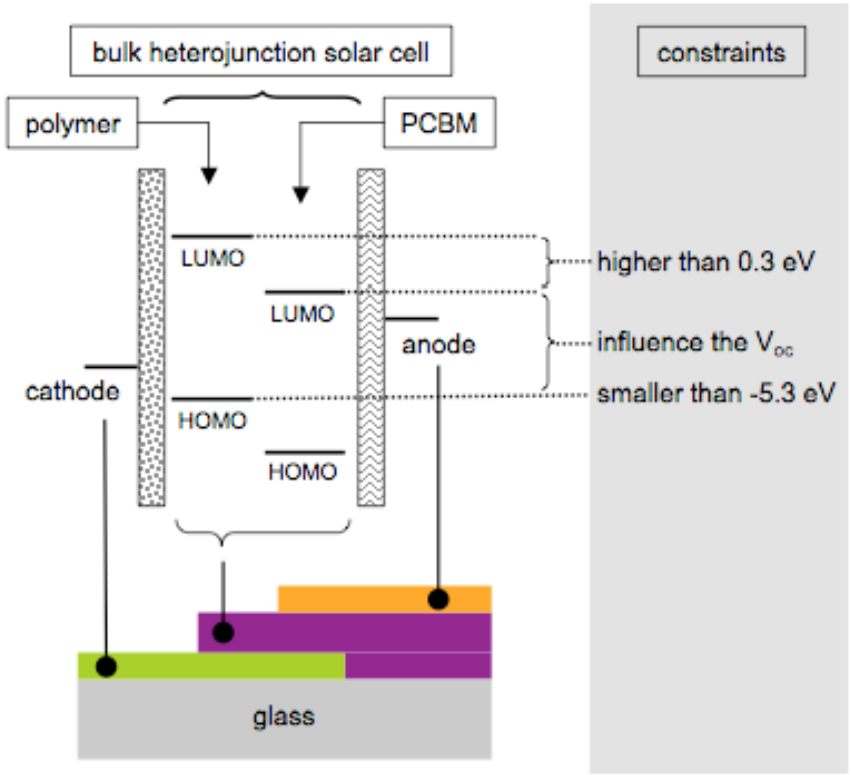
SR Bhatta et al, 2013

- Suggest a large dipole moment

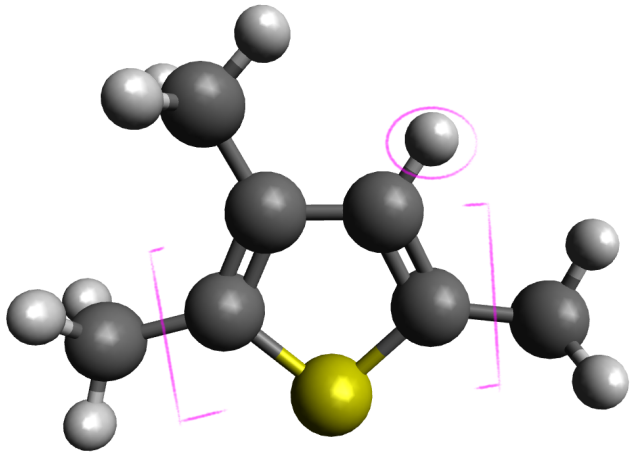
B Castern et al, 2011

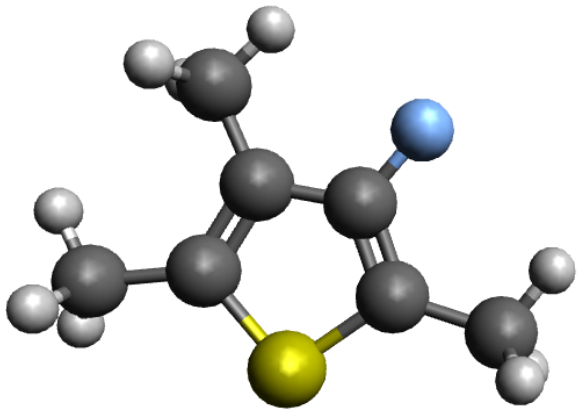
- Dipole should be aligned in a specific direction

J.F Laprade et al, 2011



Design of Polymer Solar Cells using Substitutes





Substitute hydrogen using;

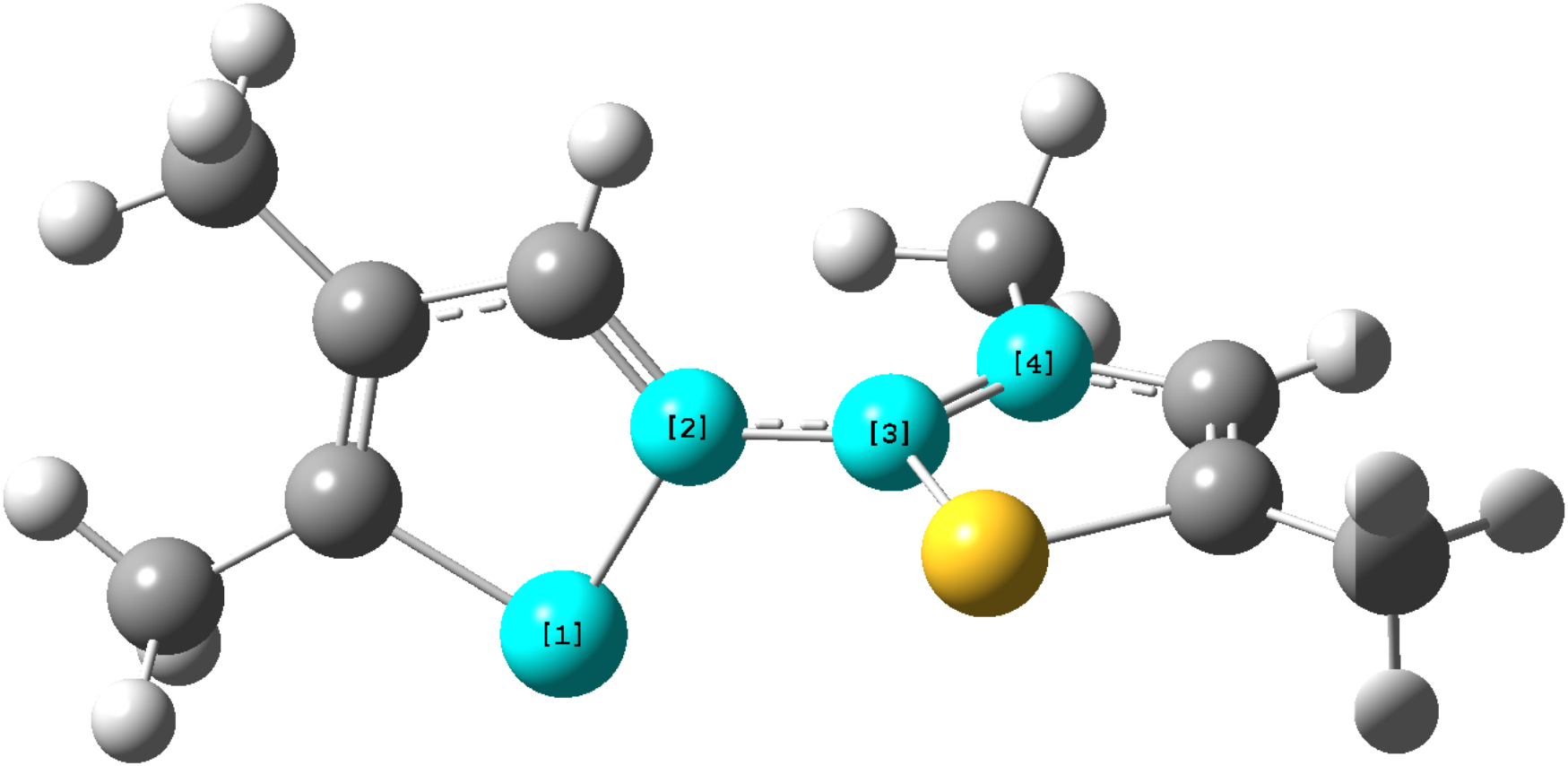
Electron Withdrawing
(-F, -Cl, -CN, -COCH3, -NO2, -COCl, -COOH, -CCL3 and -CONH2)

Electron Donating;
(-OH, -NH2, -OCH3, -CHCH2, -NHCH3, -NHOCH3, -OCOCH3 and -N(CH3)2)

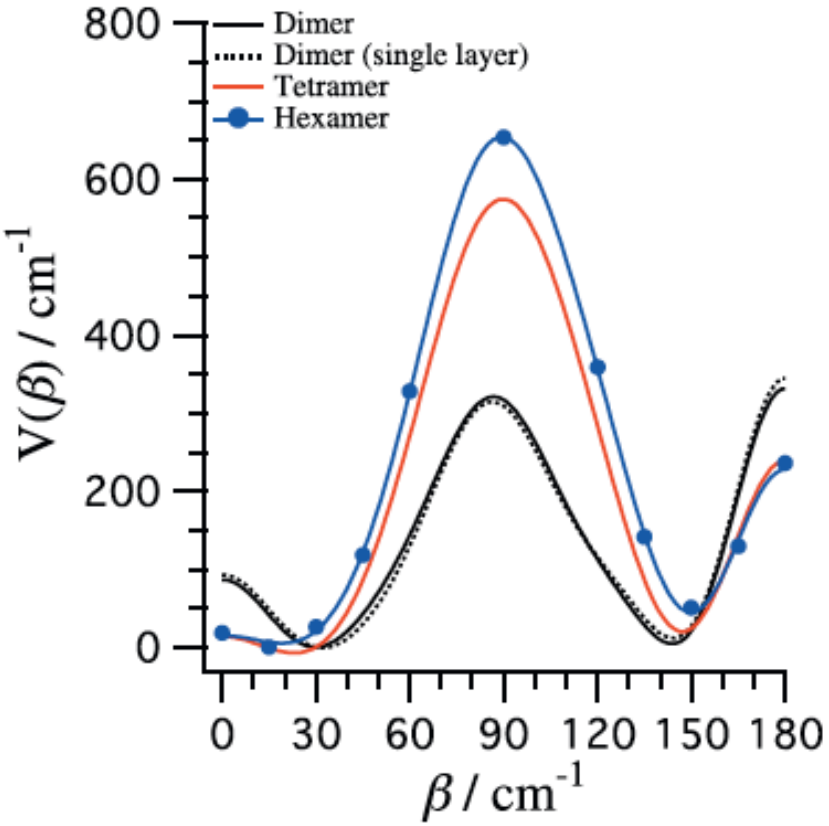
Computational Methods

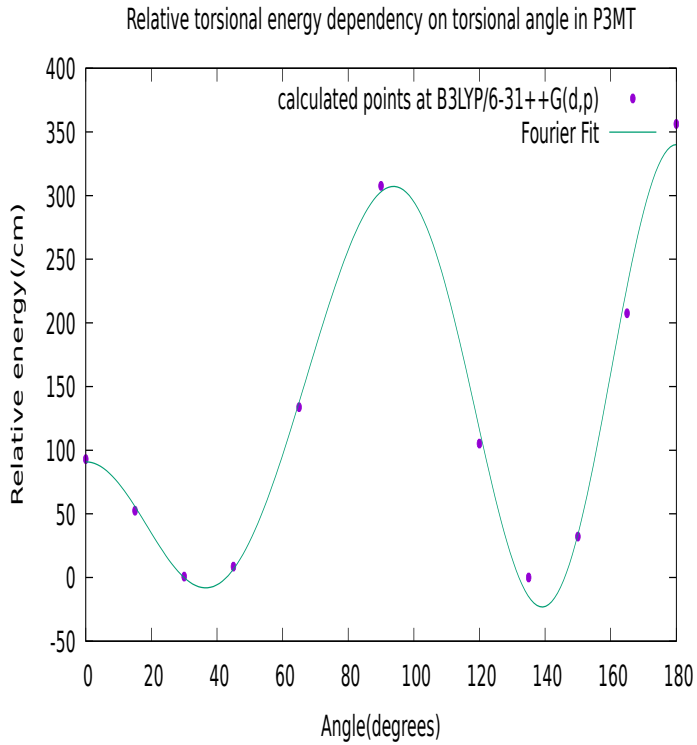
- DFT
  - △ Cost efficiency
- Nwchem_6.6 and *Gaussian_09*
  - △ Good scalability
- B3LYP/6-31G(d) and B3LYP/6-31++G(d,p)

Poly 3-methyl thiophene dimer

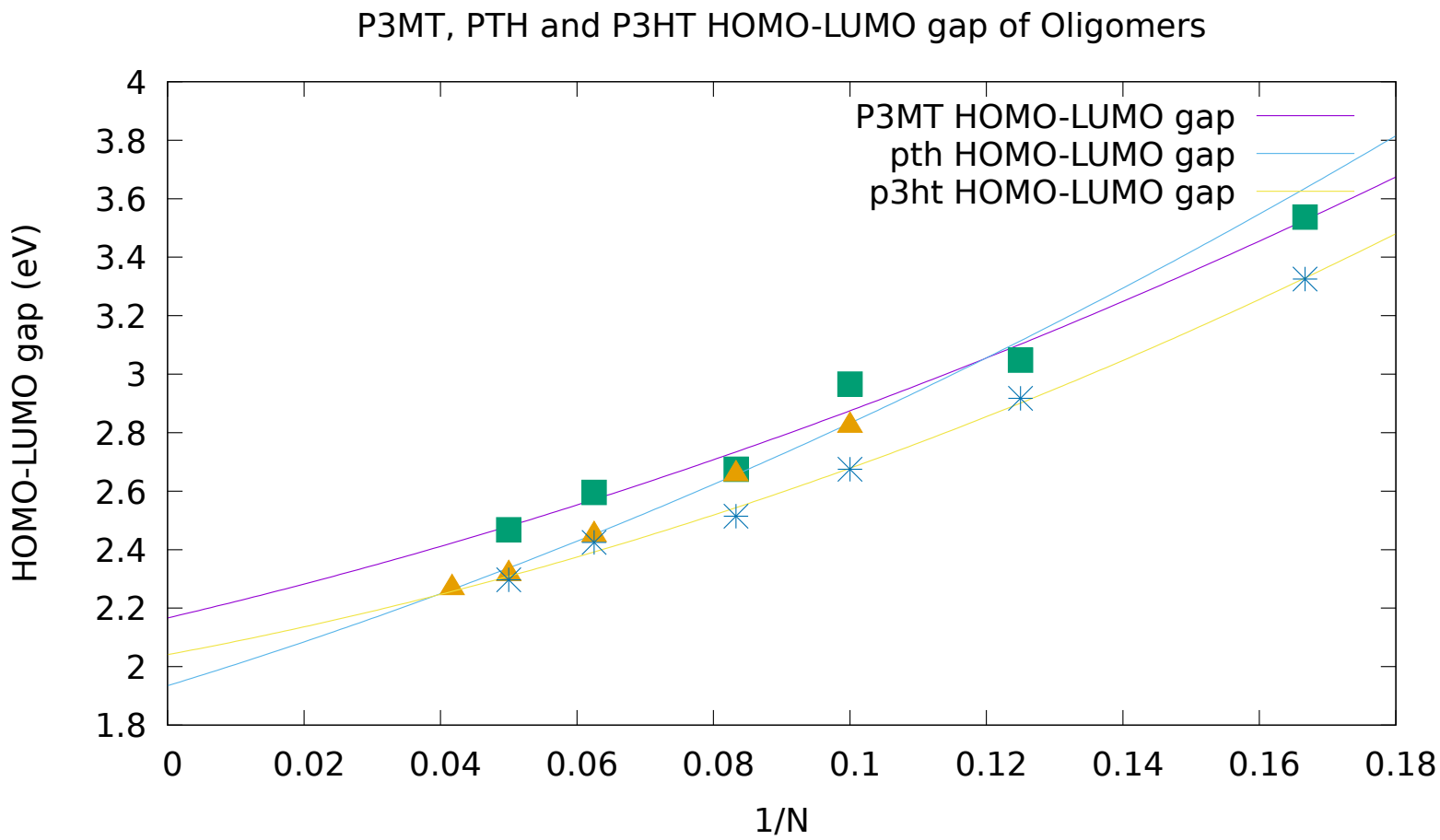


Test Calculations





Test Calculations; HOMO-LUMO gap

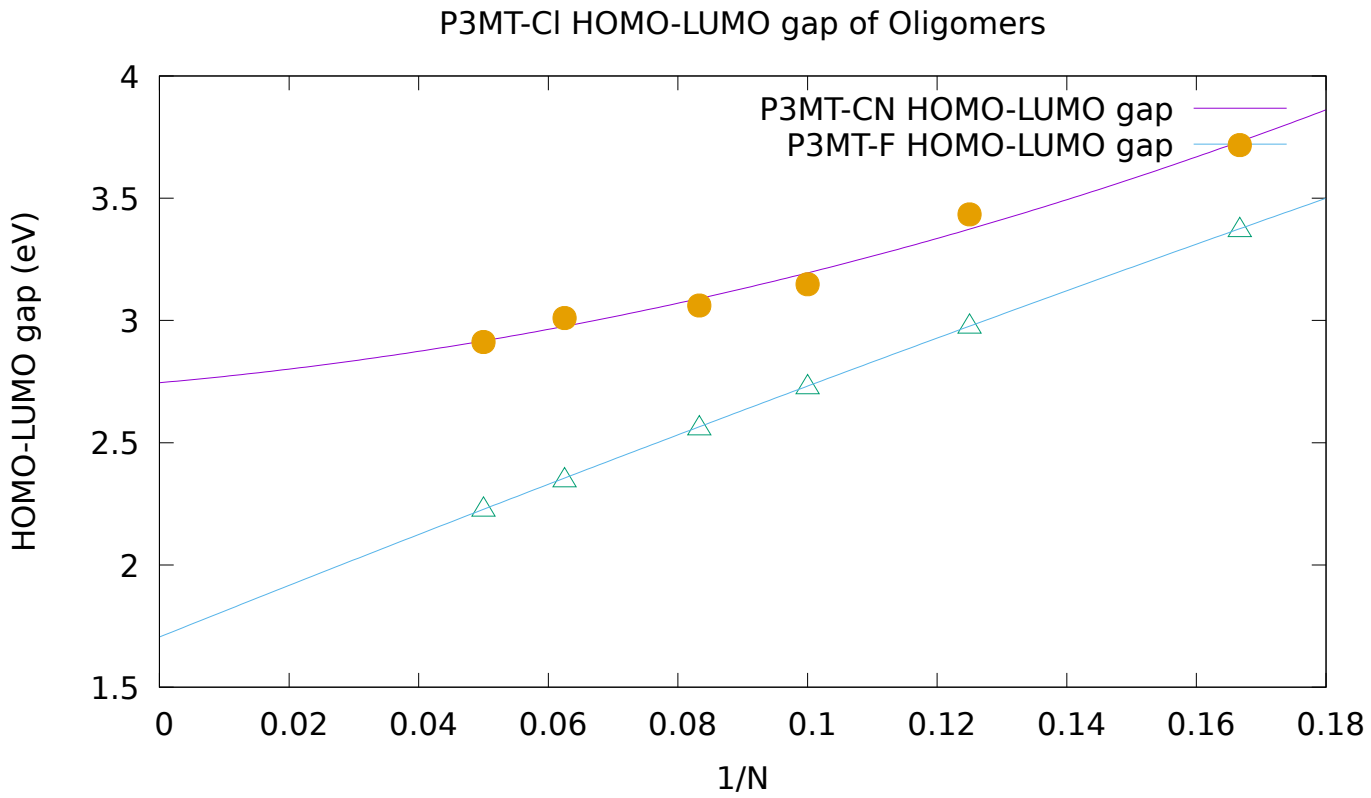


Polymer	Experimental value	Calculated value	% error
PTH	2.20	1.93	12
P3MT	2.26	2.17	4
P3HT	2.25	2.04	9

HOMO-LUMO energy gap for Monomers

Electro Withdrawing		Electron Donating	
Substitute	Gap (eV)	Substitute	Gap (eV)
-NO2	4.2	-NH2	4.76
-COCl	4.4.58	-CHCH2	4.92
-COH	4.67	-NHCH3	5.07
-COCH3	4.76	-OH	5.11
-CCl3	4.83	-N(CH3)2	5.16
-COOH	5.07	-NHOCH3	5.27
-CONH2	5.17	-OCH3	5.35
-CN	5.20	-H	5.51
-Cl	5.48	-	-
-F	5.56	-	-

HOMO-LUMO energy gap for Oligomers



Substitute	Monomer Gap (eV)	Polymer Gap (eV)
-CN	5.2	2.75
-F	5.56	1.71

Conclusions and Future plans

Conclusions

• B3LYP/6-31G(d) gives a HOMO-LUMO gap that is close to experimental value for P3MT, PTH and P3HT.

⧫ error $\leq 15\%$

• A smaller HOMO-LUMO gap is achieved with flourine substituent.

• B3LYP/6-31++G(d,p) gives an excellent agreement with experiment when calculating relative torsional energy of P3MT dimer.

Future Plans

• Calculation of HOMO-LUMO gaps when using other substituents.

• Relative torsional energy for designed molecules.

Thank You!