The Effect of Substituent Side Chain Length and Solvent Induced Transformations of Unimer to Aggregates in Polythiophene Solutions Experiment

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**ABSTRACT**

- We study solution unimer plus aggregates (P3HT, P3OT, and P3BT) that are controlled by inducing in solutions
- Good Solvent solubilizes polythiophene
- Bad Solvent induces formation of aggregates
- Control of aggregate formation by volume ratio
- Characterize unimer and aggregates of good/bad solvents by optical spectroscopy of UV-Absorption spectrum and photoluminescent spectrum

**EXPERIMENTAL PROCEDURES**

- Dissolve P3HT, P3OT, and P3BT in Chloroform (Good Solvent)
- Add control amount of bad solvents (acetone, acetonitrile, dimethylformamide, ethanol, hexane, methanol, and tetrahydrofuran)
- Measure UV-Vis absorption spectrum and photoluminescent spectrum
  - Band Gap
  - HOMO-LUMO (High Occupied Molecular Orbital and Low Unoccupied Molecular Orbital)
  - π-π stacking
- Energy Diagrams:

**P3HT IN CHLOROFORM/ACETONE**

- Absorbance (λ): 450 nm
- Absorbance (λ): 575 nm

**P3OT IN CHLOROFORM/ACETONE**

- Absorbance (λ): 450 nm
- Absorbance (λ): 570 nm

**P3BT IN CHLOROFORM/ACETONE**

- Absorbance (λ): 400 nm
- Absorbance (λ): 570 nm

**CONCLUSIONS**

- Shift of Absorption peak position from 455 nm for P3BT to 450 nm for P3HT to 455 nm for P3OT
- Maximum of Photoluminescence peak from 570 nm for P3BT down to 575 nm for P3HT to 570 nm for P3OT
- P3HT requires least amount of acetone for aggregate formations
- P3OT requires most amount of acetone for aggregate formations

**REFERENCES**