Polymorph Screening at Surfaces in an Organic Semiconductor

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Introduction

Project title: **Ultra-high Charge Carrier Mobility to Elucidate Transport Mechanisms in Molecular Semiconductors (UHMob)**

→ Substrate induced polymorphism: Origin, stability and applicability (ESR 8)

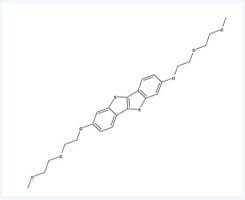
Goal: Organic semiconductor-based devices with improved charge transport properties

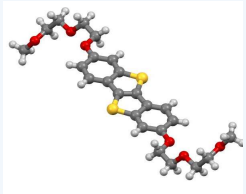
Methodology: Structure-Property relationship

Area of Investigation: 1) Design and synthesis of novel organic semiconductors
2) Charge transport studies
3) Discovery of new polymorphs

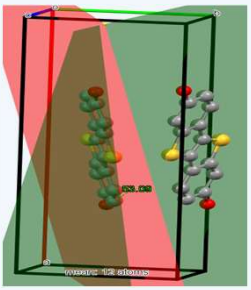
Molecule of Interest: OEG-BTBT-OEG

- Crystal structure solution





a	18.635
b	7.6670
c	8.2930
α	90
β	99.35
γ	90
Volume	1169.14
Z	2
Crystal density	1.354 g/cm^3
Temperature	298K



Herring bone angle = 53°

Thin film-forming properties

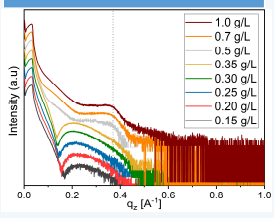
- Mono to bulk layer

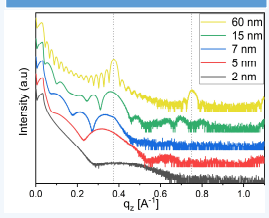
Thin film

Solution processing (spin coating)

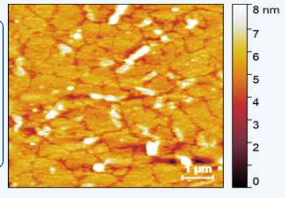
Physical vapor deposition (thermal evaporation)

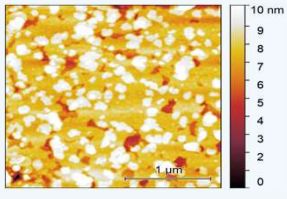
X-Ray Reflectivity



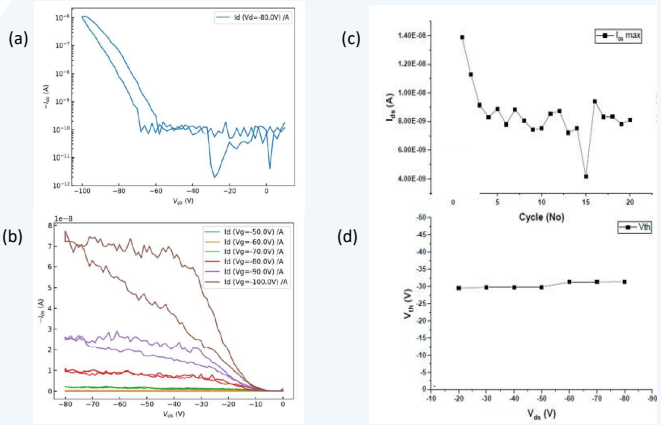


Atomic Force Microscopy



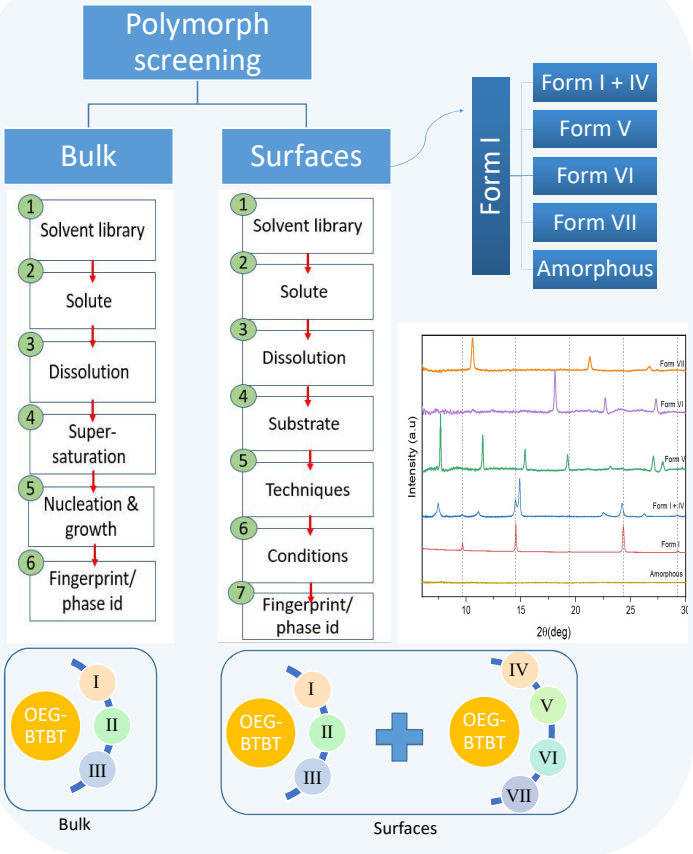


Charge transport properties



(a)Transfer and (b) output characteristics of OEG-BTBT based OFET device, (c)Maximum drain current of FD44 based transistor upon repetitive recording of transfer characteristics (V_g=-40 V, V_d=-10 V),(d) evolution of threshold voltage upon increasing V_{ds} (V_g=-40 V)

Discovering polymorphs



Conclusions

- Solved crystal structure of OEG-BTBT (Form I).
- Thin film forming properties of OEG-BTBT was investigated for solution processed and physical vapor deposited films.
- Charge transport properties of OEG-BTBT based OTFTs were studied.
- Polymorph screening process was carried out in bulk(3 phases) and at surfaces (4 phases).

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