Profiling PBTTT8O Polymer Polymorphs with Molecular Dynamics Simulations

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Background. Controlling different crystalline polymer forms (polymorphs) is essential in realizing high performance organic electronics, such as thermoelectric devices (TEs), which turn waste heat into electricity. The state-of-the-art polymer used in organic TEs is PBTTT (Fig. 1) however control over the optimal molecular packing is experimentally challenging. Currently, chemical tuning (oxygenation) of the side-chains is being explored to maximize polymer self-assembly and induce different polymorphs by the SYCOMMOR group at ICS in collaboration with ICPEES (N. Leclerc) [1]. Characterizing the structure of previously undiscovered crystalline forms is however near impossible without sub nm resolution of the polymer chains.

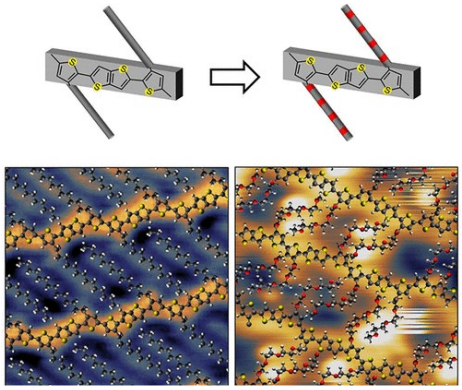

Fig 1: PBTTT & P(G2T-TT) Polymorphs under a Scanning Tunneling Microscope [2]

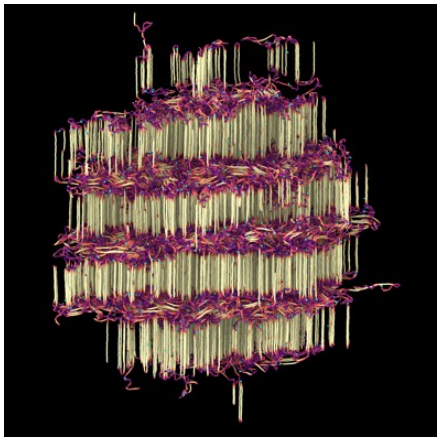

Fig 2: Multilamellar PE crystal grown by the TSP team at ICS using MD [3].

PhD Project. Molecular dynamics (MD) simulations provide a route to grow polymer crystals representative of experiments and interpret diffraction patterns from experiment. However appropriate coarse-grained models of conjugated polymers, such as PBTTT, are sadly lacking in simulations. The **Theory and Simulation of Polymers Group** (TSP) team at ICS was recently successful in growing the first large-scale multi-lamellar crystals of Polyethylene in MD simulations, see Fig. 2, using a coarse-grained united-monomer model. The aim of this project is to extend this model to PBTTT/OEG and to aid in the characterization of diffraction patterns of different polymorphs, through direct comparison with experimental structure factors (Fig. 3).

Profile. Candidates with a disposition for numerical or simulation work, a solid understanding of statistical mechanics and programming experience are highly sought after. Familiarity with LAMMPS and High-Performance computing clusters of the CNRS (Adastra/Jean-Zay) is favorable but by no means a prerequisite. The project will provide ample opportunity to interact with leading simulation experts in the TSP team as well as travel to international conferences.

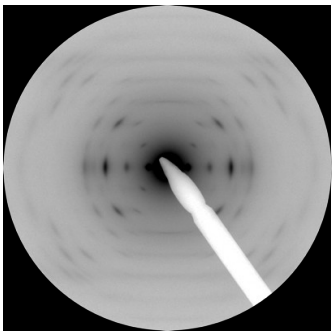

Fig 3: PBTTTOEG Diffraction pattern with unknown structure [4].

[1] Guchait, Shubhradip, et al. *Small*, 21(6), **2025**, 2410073 and P. Durand, Materials Horizons, **2024**,11, 4737-4746
[2] Moro, Stefania, et al. *ACS Nano*, 16(12), **2022**, 21303-21314.
[3] Fall, William S., et al. *ACS Macro Letters*, **2023**, 12(6), 808-813.
[4] Bilan, et al. Unpublished, **2025.**