Validating Structural and Thermodynamic Properties of Nonfullerene Acceptors for Organic Photovoltaics

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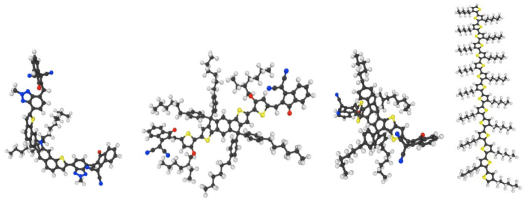
Introduction:

Organic photovoltaics (OPVs) are solar cell materials made of carbon-containing compounds that show potential in succeeding their silicon counterparts due to their low manufacturing costs and mass manufacturing potential. New OPV compounds lacking fullerenes are able to reach high efficiencies. However, the chemistries for the best non-fullerene acceptors are still unknown.

This work utilizes Molecular Dynamic (MD) simulations to predict OPV component morphology important for absorbing photons and converting them into electricity. Simulations allow morphologies to be predicted hours or days faster than wet labs. By analyzing the morphology obtained at different temperatures and ratios, we are able to identify the conditions at which compounds will self assemble into morphologies with efficient charge transport—a key predictor of solar cell efficiency.



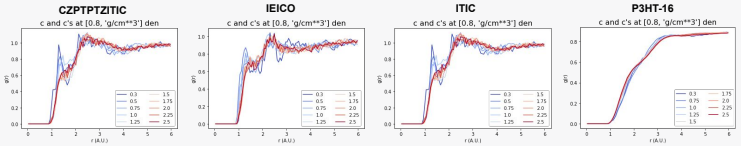
CZTPTZITIC IEICO ITIC P3HT-16

Methods:

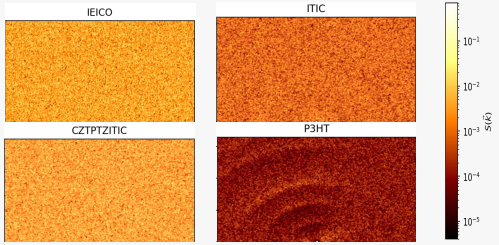
MD simulations on OPV molecules are performed using HOOMD-Blue[1] implemented in PlanckTon-Flow[2], a software package utilizing the Signac[3] framework to manage the parameter space and submit simulations. All simulations run on Fry (BSU) and Bridges2 (PSC) supercomputing clusters. We develop and automate new analyses into workflows for calculating the radial distribution function (RDF), diffraction patterns, and mean square displacements (MSD) from trajectory data.

Input parameters varied are density, temperature, and number of compounds. RDFs measure relative probability of finding two atoms a certain distance apart, normalized against a uniform distribution. Diffraction patterns allow for the determination of the stacking and ordering of the molecules. MSDs demonstrate the change of position that occur since the start of the simulation.

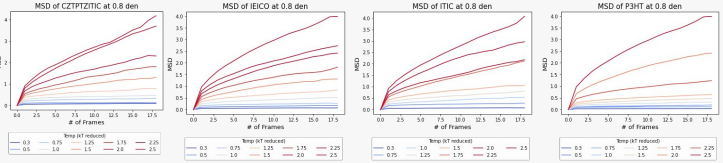
Results:



Above: The intramolecular carbon-carbon correlations quantify structural differences between molecules and temperatures. CZTPTZITIC, IEICO, and ITIC all have closer packing at low temperatures than P3HT and show more variation with temperature, despite being more disordered.

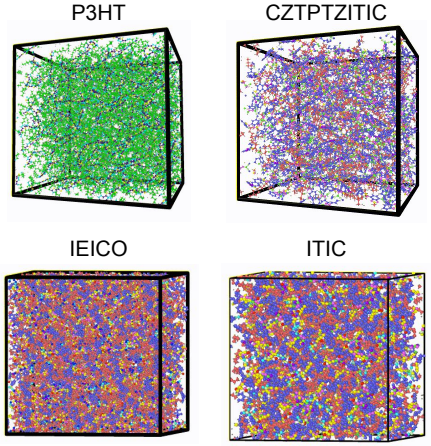


Above: Diffraction patterns of carbon atoms on the backbone of each molecule show long range organization that is or is not present in the molecule packing. CZTPTZITIC, IEICO, and ITIC are all amorphous so it is expected that nothing is seen in their diffraction patterns. P3HT, on the other hand, settles into a lamellar structure that is visible in the diffraction pattern.



Above: MSDs of all atoms in each molecule are generated at a density of 0.8 g/cm^2 with various temperatures. Runs around 0.5 kT have a dynamical slowing down of the molecules, indicating they may have passed below their glass transition temperature. Runs above 2.0 kT have a steep slope value which indicates that the molecules have surpassed their glass transition temperature causing them to move more flexibly.

Simulation:



Conclusions and Future Work:

With the techniques outlined in the methods section, it has been shown that the self-assembly and resultant morphology of organic semiconducting compounds can be predicted accurately across an array of thermodynamic state points. The morphologies obtained with this workflow show early qualitative agreement with the structural transition temperatures of P3HT and ITIC observed experimentally.

Next steps include using our new workflows to screen hundreds of candidate parameters and blends, and using their morphologies to predict the characteristics that optimize OPV performance. Having obtained these morphologies and tuned the analytical tools discussed in the results, further sanity checks can be performed to validate their quantitative characteristics. For example, charge mobility can be calculated with MorphCT (software created by our lab), which leverages Marcus Theory and Kinetic Monte Carlo simulations.

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[1] http://glotzerlab.engin.umich.edu/hoomd-blue/ [2] https://github.com/cmelab/planckton-flow [3] https://docs.signac.io