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Using Computational Tools to Accelerate Discovery of High-Efficiency Solar Cell Materials

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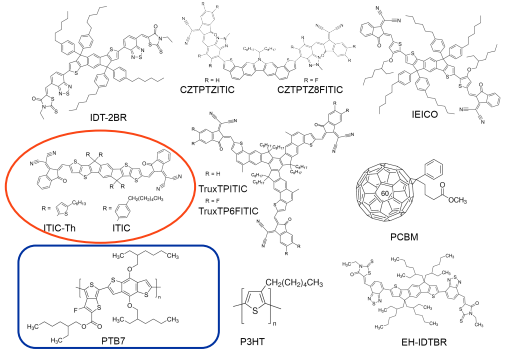
Introduction

Organic photovoltaics (OPVs) could potentially be the lowest-cost solar power generating technology. But this depends on finding the right molecules that can thermodynamically assemble arrangements that are favorable for generating power.

We take a computational approach to predict the structures of promising OPV mixtures, including non-fullerene acceptors, enabling their stable structures to be evaluated for power generation capabilities later.



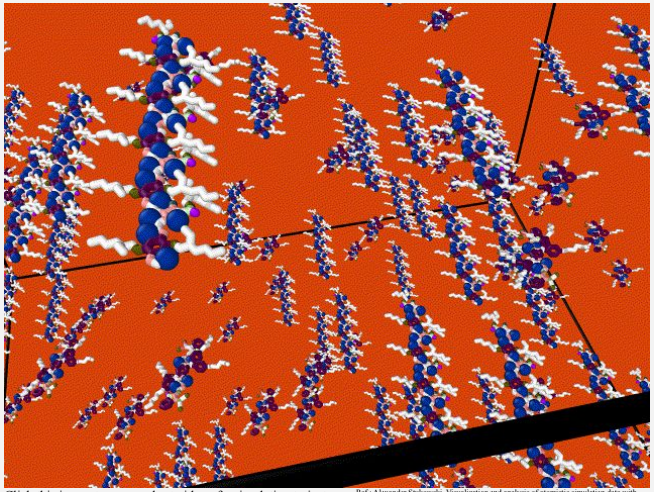
Methods:

We develop PlanckTon, which leverages the Signac framework to manage parameter spaces and job submission to high performance computer clusters and MosDeF tools to aid the initialization of **Molecular dynamics (MD)** simulations. MD simulations were performed using the HOOMD-Blue simulation engine which allows the observation the thermodynamic evolution of a system over millions of time steps. After equilibration, detailed analyses of molecular packing and potential for converting light into electricity can be performed.

To analyze molecular packing, **radial distribution functions (RDFs)** are used to measure spatial correlations between simulation elements and help to distinguish between ordered, repeatable structures and unordered, amorphous structures. The RDFs shown are calculated using the freud analysis package.

Our workflow links processing parameters (e.g., temperature, density, polymer size), equilibrium structure, and potential for power generation.

Reproducible, programmatic simulation initialization and submission helps us do better science!



Click this image to open a short video of a simulation trajectory.

Ref: Alexander Stukowski, Visualization and analysis of atomistic simulation data with OVITO-the Open Visualization Tool, MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING 18 (2010), no. 1, DOI 10.1088/0965-0393/18/1/015012.

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Results:

Representative diagnostics of PTB7 (electron donor), ITIC (electron acceptor), and PTB7:ITIC mixture simulations from thousands of HPC jobs reveal the length scales of local packing (1 AU = 1 sulfur diameter = 3.6 Angstroms)

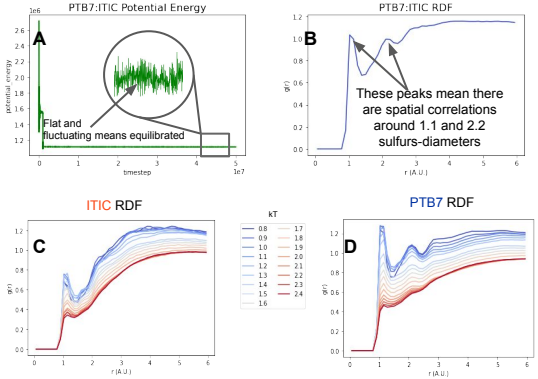

Figure A: Potential energy vs time for PTB7:ITIC at T= 0.9kT and ρ= 0.9 gm/cm^3 .
Figure B: Molecular center RDF of mixed PTB7 and ITIC have two local maxima indicating two length-scales around which these molecules are most likely to arrange with each other
Figure C: Center-center RDFs of pure ITIC show these molecules rarely have centers in contact and that both long- and short-range correlations increase with lower temperature.
Figure D: Center-center RDFs of pure PTB7 show more local ordering than ITIC and a sharper increase in local structure around T<=1.4, where g(r=1)>1.0

Conclusions:

Automating workflows enables the submission of thousands of jobs, from which slices of pure and mixed morphologies can more easily be extracted for analysis of equilibrium structure in terms of temperature and density. Here we focus on PTB7:ITIC mixtures and find their RDFs are a convolution of pure-component RDFs, each of which show ordering transitions at lower temperatures.

Future Work: Now that we have identified these ordering transitions we can perform more expensive charge-transport calculations and scattering analysis to measure how the performance of PTB7:ITIC OPVs will depend on the temperatures at which they are manufactured.