Computational Study of Solvents and Anti-Solvent Blends on the Crystallization of Hybrid Organic-Inorganic Perovskite Solar Cells.

Sponsor: Prof. Paulette Clancy, in collaboration with Prof. Joshua Choi (U.Va.).

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One or two MS students, or a team of 1-2 M.Eng. students, with variable credit of 3-4 credits in the fall and 3-4 credits in the spring.

Power conversion efficiencies of hybrid organic-inorganic perovskite (HOIP) solar cells now rival those of traditional silicon-based solar cells. Unlike silicon, HOIPs can be processed directly from solution, leading to low-cost and energy-efficient fabrication. While many studies have shown that the composition of these solutions ultimately affects the cell's efficiency, the underlying physics governing the solution processing of the final crystalline product is very poorly understood. It is also under-investigated due to the overwhelming complexity of the system that limits the coverage of possible outcomes using either a systematic or a random trial-and-error approach. Our work has investigated the driving forces of lead solubility, and complexation of the lead-salt to the B-site cation in solution. We have identified two competing design criteria to maximize two separate events that occur simultaneously; The Mayer bond order as a metric for solubility, and the relative dielectric for complexation of perovskite crystallites. This project uses Molecular Dynamics (MD) and Density Functional Theory (DFT) to study the effect of complexation and early nucleation of perovskites in solution. This project will look at the various interactions between bath solvents and anti-solvents, and how these solutions interact with the perovskite building blocks, either to promote or hinder complexation by studying electronic properties of the systems. This is a collaborative project with Prof. Joshua Choi's experimental group at the University of Virginia and Prof. Lara Estroff. We will teach students DFT and MD techniques, but the project is better suited to students with some programming skills (C, C++, python etc.) and enthusiasm for coding.