Molecular Morphology in Organic Electronics: Strategies for Simulating Charge Transport and Electronic Structure and for Depositing Ordered Phases from Chemical Solutions

Sean Shaheen

Dept. of Electrical, Computer, and Energy Engineering
Associate Professor by Courtesy, Dept. of Physics
Fellow, Renewable and Sustainable Energy Institute (RASEI)
University of Colorado Boulder

Solution processing of pi-conjugated polymers and smaller molecules takes advantage of molecular self-assembly forces and the kinetics of their solidification to produce the final morphology. This in turn determines the energetic and spatial distributions of the electronic Density of States (DOS) that underlie charge carrier transport. Here I will discuss our efforts in simulating charge carrier hopping in disordered molecular solids in the presence of spatial correlations, through a seeded-nucleation approach that mimics the physical solidification process. Next, I will present recent results on calculating a physically realistic DOS from assemblies of molecules determined by multiscale simulations, starting with Molecular Dynamics (MD) to find the molecular morphology followed by a fragment basis tight binding method for approximating the electronic eigenstates and complete DOS. Finally, I will discuss our recent experimental efforts to deposit ordered, microcrystalline thin films from chemical solutions of organic molecules, in this case C60, which do not exhibit liquid crystalline phases but can result in crystalline regions with length scales of 10’s of microns.

Wednesday, November 20th at 1:30 p.m. in Duane Physics G126