Investigating degradation pathways in organic solar cell materials

Thin film organic solar is a recent technology with tremendous potential – low cost materials, quicker manufacturing processes and synthetic tuning of organic materials to optimize material properties. Cell efficiencies > 12% have already been achieved. But the bottleneck problem this technology faces is instability. Performance of these cells degrades much faster than traditional solar cells. The degradation occurs on exposure to solar radiation, both through extrinsic ingress of moisture and oxygen as well as intrinsic degradation mechanisms.

One of the most common type or thin film organic cell with efficiency ~10% is PTB7:PCBM organic solar cell. Hence I have tried to attack the instability problem for this cell. The first step is to understand why and how the degradation occurs. Hence I have studied both extrinsic and intrinsic degradation pathways for this cell .Through theoretical simulations using quantum mechanical methods, I have tried to calculate energy barriers for possible degradation pathways, narrowing their search. Next, I try to determine the atomistic mechanisms of degradation by light-soaking organic films in controlled environment and performing infrared spectroscopy before and after light soaking, to identify bonding changes. Infrared spectroscopy paired with ab-initio theoretical modeling can provide a powerful tool for quantifying photo-structural atomic bonding changes.

Understanding these pathways, it will be easier to synthetically tune organic materials much less prone to degradation, solving the bottleneck problem of instability for thin film organic solar cells and opening avenues to designing more stable organic materials for organic electronics.