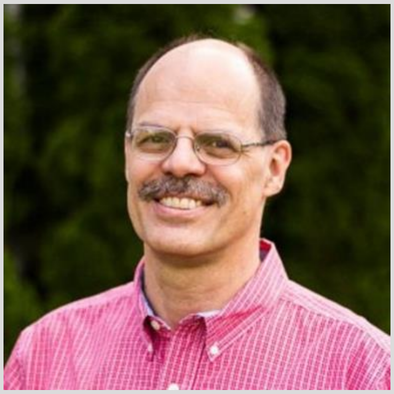
Physical Chemistry Seminar

Prof. Harald Ade

North Carolina State University

"Interplay of Microstructure and Thermodynamic in the Performance and Stability of Organic Solar Cell"



Efficiencies of close to 20% have been achieved now efficiency of organic solar cells (OSCs), making this a viable alternative for some power-conversion applications. Although the morphological stability of these of non-fullerene small-molecule acceptors (NF-SMAs) devices critically affects their intrinsic lifetime, their fundamental intermolecular interactions and how they govern property–function relations and morphological stability have remained elusive. The presentation will discuss the use of Resonant Soft X-ray Scattering (R-SoXS), Gracing Incidence Wide Angle X-ray Scattering (GIWAXS) and measurements of the miscibility gap to more fully understand structure-processing-performance relationships and how to possibly screen materials systems. Specifically, we discuss the recent discovery that the diffusion of an NF-SMA into the donor polymer exhibits Arrhenius behavior and that the activation energy scales linearly with the enthalpic Flory-Huggins interaction parameters between the polymer and the NF-SMA. Consequently, the thermodynamically most unstable, hypo-miscible systems (high interaction parameter) are the most kinetically stabilized. In short, unfavorable interactions enable stability. We have also been able to relate the differences in the activation energy to measured and selectively simulated molecular self-interaction properties of the constituent materials that provide quantitative property–function relations that link thermal characteristics (glass transition) of the NF-SMA and mechanical characteristics of the polymer (elastic modulus) of the polymers [1]. This allows predicting relative diffusion properties and thus morphological stability from simple analytical measurements or molecular dynamic simulations.

[1] Ghasemi, M., Balar, N., Peng, Z. et al. A molecular interaction–diffusion framework for predicting organic solar cell stability. Nat. Mater. (2021). https://doi.org/10.1038/s41563-020-00872-6

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Time: 10:30 am (CT)

Host: Prof. Mark Ediger

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