CHiMaD Center for Hierarchical Materials Design

MATERIALS GENOME INITIATIVE SEMINAR SERIES

Connecting Kinetic Monte Carlo Simulations and Experimental Characterization Techniques to Elucidate Processing-Structure-Property Relationships in Nanostructured Semiconductor Devices

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Abstract: Among a variety of simulation and modeling methods covering varying length and timescales, kinetic Monte Carlo (KMC) simulations have been a uniquely powerful tool due to their ability to capture nanoscale materials morphological details while retaining the ability to simulate full devices, thereby acting as a coarse-grained model that bridges the gap between atomistic and continuum methods. In this talk, I will introduce the fundamentals of KMC simulations, overview their past and ongoing use in organic semiconductor materials and devices, and discuss potential future applications to low-dimensional materials. As examples, I will highlight my use of KMC simulations with model bulk heterojunction blend morphologies [1] to develop novel predictive physical models that capture how the complex materials microstructure impacts exciton dynamics,[2] bimolecular charge recombination kinetics,[3] and charge carrier transport.[4] To further connect these theoretical predictions to experimental observations, I will outline my current work integrating transmission electron microscope tomography data into my new open-source KMC simulation software tool [5] and discuss the development and use of a new impedance-based device characterization method for quantifying the charge recombination and transport behavior and for generating information-rich datasets for future statistical analysis and machine learning efforts.[6] This work demonstrates a unique, cross-disciplinary approach to electronic materials and device development that produces improved physical models and high-quality data to accelerate the discovery and development of new materials.

[1] M. C. Heiber and A. Dhinojwala, Phys. Rev. Appl. 2, 014008 (2014). "Efficient Generation of Model Bulk Heterojunction Morphologies for Organic Photovoltaic Device Modeling"
[2] M. C. Heiber and A. Dhinojwala, J. Phys. Chem. C 117, 21627 (2013). "Estimating the Magnitude of Exciton Delocalization in Regioregular P3HT"
[3] M. C. Heiber, C. Baumbach, V. Dyakonov, and C. Deibel, Phys. Rev. Lett. 114, 136602 (2015). "Encounter- Limited Charge-Carrier Recombination in Phase-Separated Organic Semiconductor Blends"
[4] M. C. Heiber, K. Kister, … V. Dyakonov, C. Deibel, and T.-Q. Nguyen, Phys. Rev. Appl. 8, 054043 (2017). "Impact of Tortuosity on Charge-Carrier Transport in Organic Bulk Heterojunction Blends"
[5] M. C. Heiber, Excimontec v1.0-beta, https://github.com/MikeHeiber/Excimontec (2017).
[6] M. C. Heiber, T. Okubo, … G. C. Bazan, and T.-Q. Nguyen, Energy Environ, Sci. (2018). "Measuring the Competition between Bimolecular Charge Recombination and Charge Transport in Organic Solar Cells under Operating Conditions"

Bio: *Dr. Heiber obtained a B.S. in Materials Science and Engineering at the University of Illinois at Urbana-Champaign in 2007 and a Ph.D. in Polymer Science from the University of Akron in 2012 with Prof. Ali Dhinojwala. Through his graduate studies and previous postdoctoral positions working with Prof. Vladimir Dyakonov at the University of Würzburg, Prof. Carsten Deibel at Chemnitz University of Technology, and Prof. Thuc-Quyen Nguyen at the University of California, Santa Barbara, he has developed a broad set of computational and experimental skills for investigating the physics of novel semiconductor materials and devices. His broader research interests revolve around efforts to combine multiscale simulations and advanced experimental techniques to develop physical models for emergent kinetic phenomena in complex materials system. In July 2017, he joined the Polymers Processing Group at NIST, led by Dean DeLongchamp, as a NIST-CHiMaD postdoctoral fellow where he has been coordinating an effort to combine advanced materials morphology measurements, kinetic Monte Carlo simulations, and electrical device characterization techniques to reveal the complex processing-structure-property relationships in organic solar cells.*