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## Determining Molecular Orientation, Packing, and Domain Purity in Organic Photovoltaic Devices with Synchrotron Radiation

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In bulk heterojunction (BHJ) organic photovoltaics (OPVs), electron donating and electron accepting materials form a complex network of discrete and distributed heterointerfaces and charge transport pathways in the photoactive layer where critical photo-physical processes occur. However, little is known about the structural properties of these interfaces due to their 3-dimensional arrangement and the paucity of techniques to measure local order. The presentation will review the use of synchrotron radiation based methods that can uniquely measure critical structural parameters. This includes molecular orientation relative to donor/acceptor heterojunctions [1]. Using resonant soft X-ray scattering [2], the degree of molecular orientation, an order parameter that describes face-on (+1) or edge-on orientation (-1) relative to these heterointerfaces, can be determined. By manipulating the degree of molecular orientation through choice of molecular chemistry and processing solvent characteristics, the importance of this structural parameter on the performance of BHJ OPV devices can be demonstrated. We will furthermore show how compositional variations can be related to polymer crystal size [3] and how mobility and purity can relate to charge extraction and thus in turn to device performance [4,5]. A complete description of actual morphologies and theoretical modeling yet to be developed for OPVs will have to take these factors into account.

1. J. R. Tumbleston et al., Nature Photonics 8, 386 (2014).
2. B. A. Collins et al., Nat. Mater. 11, 536 (2012).
3. W. Ma et al., Advanced Materials, 10.1002/adma.201400216 (2014)
4. S. Albrecht et al. J. Physical Chemistry Letters 5, 1131-1138 (2014).
5. Collaboration with Wei You and Dieter Neher groups, submitted.

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### Summary

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