Predicting X-ray absorption spectra of semiconducting polymers for electronic structure and morphology characterization GREGORY SU, SHRAYESH PATEL, Univ of California - Santa Barbara, C. DAS PEMMARAJU , Lawrence Berkeley National Laboratory, EDWARD KRAMER, Univ of California - Santa Barbara, DAVID PRENDERGAST, Lawrence Berkeley National Laboratory, MICHAEL CHABINYC, Univ of California - Santa Barbara — Core-level X-ray absorption spectroscopy (XAS) reveals important information on the electronic structure of materials and plays a key role in morphology characterization. Semiconducting polymers are the active component in many organic electronics. Their electronic properties are critically linked to device performance, and a proper understanding of semiconducting polymer XAS is crucial. Techniques such as resonant X-ray scattering rely on core-level transitions to gain materials contrast and probe orientational order. However, it is difficult to identify these transitions based on experiments alone, and complementary simulations are required. We show that first-principles calculations can capture the essential features of experimental XAS of semiconducting polymers, and provide insight into which molecular model, such as oligomers or periodic boundary conditions, are best suited for XAS calculations. Simulated XAS can reveal contributions from individual atoms and be used to visualize molecular orbitals. This allows for improved characterization of molecular orientation and scattering analysis. These predictions lay the groundwork for understanding how chemical makeup is linked to electronic structure, and to properly utilize experiments to characterize semiconducting polymers.

Gregory Su
Univ of California - Santa Barbara