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A Close Look at the Structure of Polymers with Soft X-rays: Insights from Theory and Experiment GREGORY SU, Lawrence Berkeley National Laboratory, SHRAYESH PATEL, University of Chicago, ISVAR CORDOVA, MICHAEL BRADY, DAVID PRENDERGAST, Lawrence Berkeley National Laboratory, MICHAEL CHABINYC, University of California, Santa Barbara, CHENG WANG, Lawrence Berkeley National Laboratory — Continued advances in the performance of polymer-based applications depends on an understanding of the connections among chemistry, structure, and dynamics in polymeric materials. These relationships are difficult to probe, especially under *in situ* or *operando* environments, and simulations are needed to unravel experimental results. We show how first-principles calculations of soft X-ray absorption spectroscopy can help understand the fundamentals of electronic structure in conjugated polymers, and elucidate structural parameters such as backbone tilt or polymer chain axis orientation. The important effects of various molecular parameters such as polymer chain length, side chain atoms, and backbone orientation on simulated spectra is demonstrated for model conjugated polymer systems. Core-level spectroscopy, which is sensitive to chemical moieties and electronic structure, is closely linked to resonant scattering that can additionally reveal spatial information. Progress in theory is also needed to connect spectroscopic and scattering techniques. The combination of these methods is evolving to probe chemistry and morphology of soft matter in a time-resolved manner.

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