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Resonant Tender X-ray Diffraction for Disclosing the Molecular Packing of Paracrystalline Conjugated Polymer Films

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The performance of optoelectronic devices based on conjugated polymers is critically dependent upon molecular packing; however the paracrystalline nature of these materials limits the amount of information that can be extracted from conventional X-ray diffraction. Resonant diffraction (also known as anomalous diffraction) occurs when the X-ray energy used coincides with an X-ray absorption edge in one of the constituent elements in the sample. The rapid changes in diffraction intensity that occur as the X-ray energy is varied across an absorption edge provide additional information that is lost in a conventional nonresonant experiment. Taking advantage of the fact that many conjugated polymers contain sulfur as heteroatoms, this work reveals pronounced resonant diffraction effects at the sulfur K-edge with a particular focus on the well-studied electron transporting polymer poly([N,N′-bis(2-octyldodecyl)-naphthalene-1,4,5,8-bis(dicarboximide)-2,6-diyl]-alt-5,5′-(2,2′-bithiophene)), P(NDI2ODT2. The observed behavior is found to be consistent with the theory of resonant diffraction, and by simulating the energy-dependent peak intensity based on proposed crystal structures for P(NDI2OD-T2) it is shown that resonant diffraction can discriminate between different crystalline packing structures. The utilization of resonant diffraction opens up a new way to unlock important microstructural information about conjugated polymers for which only a handful of diffraction peaks are typically available.

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