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Local and extended structuring in not-so-crystalline molecular solids

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One of many benefits of real-space analysis is to provide a different vantage point from which to analyze our diffraction/scattering data. Certain features of the structure are better emphasized in real-space. This provides opportunities to test different hypotheses about parts of the structure, and how they change, even when a complete structural model is unknown or not well defined. In this talk, I will discuss different case studies for using PDF data to study complex molecular materials — e.g. thiophosphate anions with dynamic disorder and macromolecular chain structures forming heterogeneous aggregations. I will show how to disambiguate aspects of the structuring over different length-scales. Importantly, emphasis will be placed on comparing total scattering features with their real-space analogues to help build intuition for future PDF endeavors.

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