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# PDF talk (xINTERPDF software)

*Monday, 7 May 2018 11:30 (25 minutes)*

Structures of organic compounds are more complex than their inorganic counterparts, which have usually a network structure, representing a giant "molecule". Organics, on the other hand, have strong intramolecular bonds but much weaker intermolecular interactions, making them prone to structural disorders. Another complexity comes from the weak X-ray scattering of light elements (C, H, O, N etc) which are the building blocks of organic compounds. The atomic pair distribution function (PDF) calculated from synchrotron X-ray total scattering has been demonstrated to be a valuable tool for investigating structures of disordered and amorphous organics compounds (Shi et al., 2017; Prill et al., 2015; Prill et al., 2016). Although existing tools such as DiffPy-CMI (Juhás et al., 2016) and XISF (Mou et al., 2015) can be used for solving this problem, a new software program is still of great value that provides a user-friendly graphical user interface (GUI, as opposed to command-driven in DiffPy-CMI) and analyzes the data in real-space (as opposed to reciprocal space in XISF). In my talk I will introduce xINTERPDF, a GUI program for analyzing intermolecular pair distribution functions in organic compounds from X-ray total scattering data. I will briefly discuss its design, distribution and application examples. The program is freely available at https://github.com/curieshicy/xINTERPDF.

References:

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