

SPS-XRPD Workshop



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PDF talk (xINTERPDF software)

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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:

- Shi, C., Teerakapibal, R., Yu, L. & Zhang, G. G. Z. (2017). *IUCrJ* 4, 555-559.
- Prill, D., Juhás, P., Schmidt, M. U. & Billinge, S. J. L. (2015). *J. Appl. Cryst.* 48, 171-178.
- Prill, D., Juhás, P., Billinge, S. J. L. & Schmidt, M. U. (2016). *Acta Crystallogr. A* 72, 62-72.
- Juhás, P., Farrow, C. L., Yang, X., Knox, K. R. & Billinge, S. J. L. (2015). *Acta Crystallogr. A* 71, 562-568.
- Mou, Q., Benmore, C. J. & Yarger J. L. (2015). *J. Appl. Cryst.* 48, 950-952.

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