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Recent advances in the magnetic pair distribution function technique

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Nanoscale magnetic correlations can be found in a variety of material systems, including strongly correlated electron materials, geometrically frustrated magnets, dilute magnetic semiconductors, and magnetic nanoparticles. Our understanding of this type of local magnetism and its role in material properties is challenged by the difficulty of experimentally probing such short-range correlations with conventional techniques, such as traditional neutron diffraction. Short-range magnetic correlations give rise to diffuse scattering rather than sharp Bragg peaks, precluding the use of the usual magnetic Bragg peak analysis commonly applied to materials with long-range magnetic order. Magnetic pair distribution function (mPDF) analysis is a newly developed neutron total scattering method that probes short-range magnetic correlations directly in real space by Fourier transforming magnetic diffuse scattering. [1] Real-space models of the local magnetic structure can then be compared directly to the data, allowing quantitative refinement of short-range magnetic correlations. Here, we discuss recent advances in the mPDF technique, particularly the ability to simultaneously acquire the atomic and magnetic PDF from neutron total scattering measurements and perform quantitative co-refinements of the local atomic and magnetic structure. [2,3] As illustrative examples, we present the results of mPDF analysis of transition-metal oxide materials, a dilute magnetic semiconductor system, and a geometrically frustrated spin glass. Finally, we briefly introduce the open-source software package diffpy.mpdf, a versatile tool for mPDF analysis and modeling created as part of the DiffPy suite of python packages for diffraction and PDF analysis.

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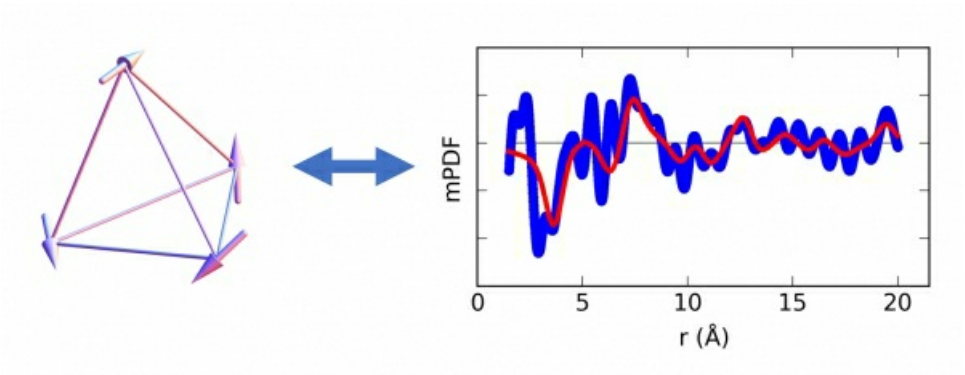

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