Real Space Mapping of Structural Correlations in Quantum Materials

Ray Osborn, Argonne National Laboratory

Although diffuse scattering is a powerful probe of short-range order in crystalline materials, its use has been limited by the experimental challenge of collecting data over sufficiently large volumes of reciprocal space and the theoretical challenge of modeling the results. However, instrumental and computational advances now allow the efficient measurement and rapid transformation of reciprocal space data into three-dimensional pair distribution functions, providing model-independent "images" of nanoscale disorder in real space. By eliminating Bragg peaks before the transformation, these 3D-ΔPDF measurements reveal structural correlations directly, displaying only the probabilities of interatomic vectors that deviate from the average structure. I will discuss two examples. In the first, 3D-ΔPDF maps reveal the collapse of 3D order at the metal-insulator transition of doped VO_2 and the emergence of extended 2D correlations resulting from a novel form of geometric frustration. In the second, structural distortions due to a charge-density-wave in $Sr_3Rh_4Sn_{13}$ are shown to persist above Tc, consistent with an order-disorder transition.

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