3D probing of hidden nanoscale states in functional materials

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Local structure in advanced materials plays an important role in unveiling the exotic functionalities and properties. The conventional one-dimensional pair distribution function (1D-PDF) method has been widely applied to studying the local structural distortions beyond the averaged crystallographic structure. However, the challenge in 1D-PDF analysis is mainly due to the powder isotropic average, which loses the directional information of atomic pairs. Here we develop the three-dimensional PDF (3D-PDF) method to resolve this problem. The experiment collects total scattering signals from a single crystal sample, and the experimental data can be reconstructed in the full 3D space. In this way, the interatomic distance vector information is retained, which can be further analyzed quantitatively using our newly developed 3D-PDF software. This method has been successfully applied to some complex functional materials, such as those exhibiting ultralow thermal conductivity and superionic behavior.[1-3] The 3D-PDF total scattering experiment is capable of retrieving diffuse scattering in a straightforward way, which can be widely applied to revealing the local atomic structural features of various materials.

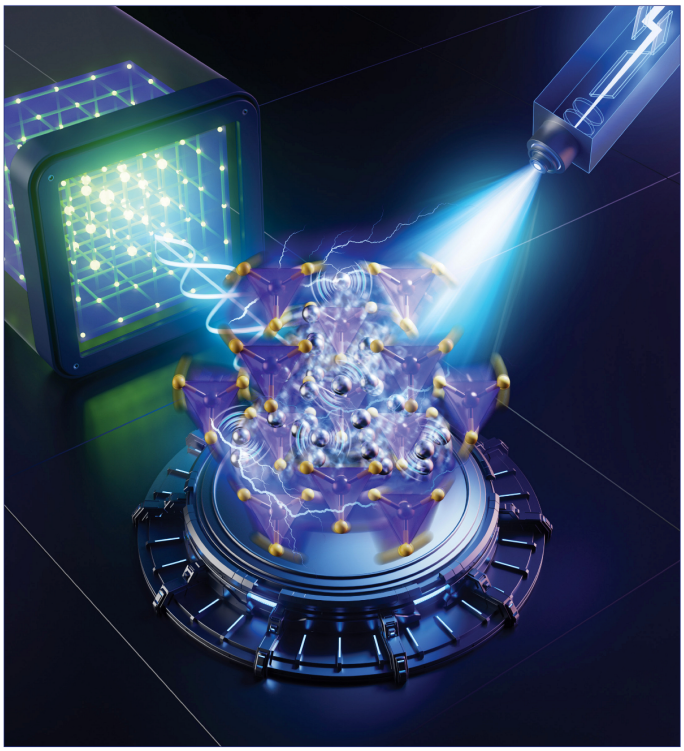


Figure 1. *The 3D-PDF total scattering experiment has been implemented in functional materials.*

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[2] C. Li, D. Zhang, X. Zhang, H. Zhang, J. Cheng, Z. Chen, H. Lin, X. Meng, W. Li, and **L. Yang***. Nanoscale local symmetry optimization induced low lattice thermal conductivity in I-V-VI2 compounds, Adv. Funct. Mater., (2026). e74755. https://doi.org/10.1002/adfm.74755.
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