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Elucidating 2D Charge-Density-Wave Atomic Structure in an MX–Chain by the 3D-ΔPair Distribution Function Method

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Abstract

Many solids, particularly low-dimensional systems, exhibit charge density waves (CDWs). In one dimension, charge density waves are well understood, but in two dimensions, their structure and their origin are difficult to reveal. Herein, the 2D charge-density-wave atomic structure and stabilization mechanism in the bromide-bridged Pd compound [Pd(cptn)2Br]Br2 (cptn=1R,2R-diaminocyclopentane) is investigated by means of single-crystal X-ray diffraction employing the 3D-Δpair distribution function (3D-ΔPDF) method. Analysis of the diffuse scattering using 3D-ΔPDF shows that a 2D-CDW is stabilized by a hydrogen-bonding network between Br^- counteranion and the amine (NH_2) group of the cptn in-plane ligand, and that 3D ordering is prevented due to a weak plane to plane correlation. We extract the effective displacements of the atoms describing the atomic structure quantitatively and discuss the stabilization mechanism of the 2D-CDW. Our study provides a method to identify and measure the key interaction responsible for the dimensionality and stability of the CDW that can help further progress of rational design.

References

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