# Combined EXAFS and X-ray Pair Distribution Function (XPDF) analysis of local structure in calcium carbonates and ferroelectric relaxors

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Extended X-ray absorption fine structure (EXAFS) and X-ray Pair Distribution Function (XPDF) analysis are versatile complementary techniques that provide information about local structure and bonding in crystalline and non-crystalline materials. Both techniques provide information about the coordination number of neighbouring atoms, bond distances and the degree of static/thermal disorder. EXAFS is a well-established element-specific method that provides short-range order information around the X-ray absorber of interest. XPDF is not element-specific, but provides short-range order information similar to EXAFS, alongside long-range structure.

EXAFS has previously been extensively used to characterise the structure of the calcium carbonate ($CaCO_3$) polymorphs, calcite, aragonite and vaterite. Structural elucidation of these polymorphs using EXAFS has been inconclusive due to limited accuracy in estimating inelastic and multiple scattering contributions. This is evident through inconsistencies in fitting the EXAFS beyond the first Ca-O shell. Our EXAFS/XPDF analysis of $CaCO_3$ accounts for multiple scattering effects and determines structural information beyond a distance of 6 Å. Our results also highlight the sensitivity of XPDF to variations between proposed crystal structure models especially with metastable vaterite, whose crystal symmetry, unit cell dimensions and orientation of the carbonate ions are controversial.

We also report a comparative EXAFS/XPDF study of the temperature-dependent structure of the ferroelectric relaxor material BCT-BMT, which is composed of a solid solution of Ca-doped $BaTiO_3$ and $Bi(Mg_{0.5}Ti_{0.5})O_3$. This relaxor is a candidate for ferroelectric capacitors suitable for applications at high temperatures. Changes in local polar nanostructure occur as a function of temperature and their quantification provides a deeper understanding of the structural origins causing the dielectric variations.

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