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ABSTRACT:

Structural Aspects of the Superionic Transition in AX_2 Compounds with the Fluorite Structure

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Some AX_2 binary compounds with the fluorite structure (space group Fm3m) are well known examples of materials exhibiting transitions to ionic superconducting phases at high temperatures below their melting points. Such superionic states have been described as either highly defective crystals or part-crystal, part-liquid states where the A ions retain their crystalline order whilst the X ions undergo partial melting. However, no detailed description of the structure of these phases exists. We present here the results of our investigation of the structural changes that occur during these transitions and the structural characteristics of the resulting superionic materials. This work [1] is based on atomic-scale molecular dynamics modelling methods as well as computational diffraction techniques. We employed a set of empirical potentials representing several compounds with the fluorite structure to investigate any potential-dependent effect. We show the importance of small-scale structure changes, with some local environments showing a hexagonal symmetry similar to what is seen in the scrutinyite structure that has been documented for example in UO_2.

[1] P.C.M. Fossati, A. Chartier, and A. Boulle, Front. Chem., 9, 723507 (2021).