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PLENARY LECTURE

Symmetry assisted insights into functional materials

Mark Senn

I will give an overview of how I have used symmetry in my work to aid in the interpretation of the often complex diffraction patterns and structures that arise as a result of phase transitions driven by electronic, ferroelectric and soft mode instabilities. I will show that a symmetry motivated ("distortion mode") basis provides not only the natural coordinate system in which to refine such powder diffraction data, but how, in the case of the topical hybrid improper ferroelectric $Ca_3Ti_2O_7$, its application leads to a deeper understanding of the soft mode physics that underpin this novel ferroic mechanism.[1] These insights have also enabled us to rationalise the occurrence of negative thermal expansion (NTE) that occurs in phases that compete with, and suppress, this ferroelectric state.[2] Ultimately we have been able to use this understanding to tune and enhance the magnitude of uniaxial NTE in a range of layered perovskites.[3] I will go on to show how a symmetry motivated basis can also be used to analyse pair distribution data in order to extract information relating to disorder. In the case of the archetypal ferroelectric $BaTiO_3$, I will show that our results firmly evidence an order-disorder nature for the phase transitions in this material, with off-centre displacements persisting well into the paraelectric state.[4] Equally, this approach to analysing PDF data provides a means for extracting information on dynamic displacements related to soft modes, which I will illustrate for a variety of perovskites that display NTE. Finally, I will show how this symmetry motivated basis can give us predictive power, enabling us to propose a scheme for designing materials with novel ferroelectric and magnetoelectric couplings.[5]

1)Negative Thermal Expansion in Hybrid Improper Ferroelectric Ruddlesden-Popper Perovskites by Symmetry Trapping. Mark S. Senn et al. Phys. Rev. Lett. 114 (2015), 035701. 2)The origin of uniaxial negative thermal expansion in layered perovskites. Chris Ablitt, et al. npj Computational Materials 3 (2017), 44. 3)Symmetry Switching of Negative Thermal Expansion by Chemical Control. Mark S. Senn, et al. J. Am. Chem. Soc., 138 (2016), 5479. 4)Emergence of long-range order in BaTiO3 from local symmetry-breaking distortions. Mark S. Senn, et al. Phys. Rev Lett. 116 (2016), 207602. 5)A Group-theoretical Approach to Enumerating Magnetoelectric and Multiferroic Couplings in Perovskites. Mark S. Senn, Acta Crystallogr. Sect. A 74 (2018), 308.

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