

Examination of local distortions and long-range polarity in pyrochlore oxides through total scattering techniques

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Oxides that crystallize in the pyrochlore structure exhibit many of the favorable properties of the leading polar perovskite materials: stability at high temperatures, ease of preparation, and flexibility to chemical substitution. This complex structure consists of two interpenetrating metal oxide networks, and exhibits a wide variety of functionalities. However, due to the triangular arrangements of cations on the pyrochlore lattice, off-centering of cations is frustrated, inhibiting the ferroelectric-paraelectric phase transition in majority of pyrochlore oxide materials. Some pyrochlore materials can overcome this frustration and exhibit polar crystal structures, and unraveling the origin of such leads to the understanding of polarity in complex materials. This work will discuss variations in crystallographic polarity and underlying local distortions across families of pyrochlore materials, including the flagship ferroelectric pyrochlore $\text{Cd}_2\text{Nb}_2\text{O}_7$, the anion deficient nonpolar $\text{Pb}_{1.5}\text{Nb}_2\text{O}_{6.5}$, and the "charge ice" $\text{Bi}_2\text{Ti}_2\text{O}_7$. We investigate the intrinsic nature of the compounds, as well as changes in polar behavior upon substitution onto either of the interpenetrated networks in the pyrochlore structure. Compositions are investigated through synchrotron X-ray total scattering, neutron total scattering, and density functional theory. This work provides insight into the complex structural behavior of pyrochlores, and informs on the relationship between local polar regions and long-range polarity in frustrated materials.