Physicists' work deepens understanding of antipolar cation motions

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University of Arkansas physicists studying antipolar cation motions found new features that deepen the knowledge on this intriguing effect. The study, by physics graduate student Kinnary Patel, research professor Sergey Prosandeev and Distinguished Professor Laurent Bellaiche, was published in August in the journal *npj Computational Materials*.

Antipolar materials are receiving a lot of attention because they are both fundamentally intriguing and technologically promising as precursors to high-energy devices. Antipolar atomic motions present an intriguing antiphase displacement of charged ions in the crystal lattice along a specific axis. The reasons for these motions are not fully understood. There are strong debates and different models to explain such motions.

Most studies devoted to this strange effect have focused on the static properties of these intriguing materials. In contrast, the article by Kinnary Patel et al considers dynamical properties associated with antipolar motions by performing multiprocessor computations at the University of Arkansas' High Performance Computing Center. U of A researchers revealed that such motions occur below a certain critical temperature because of a subtle coupling with other structural degrees of freedom that desire to have unstable vibrations below this temperature. The authors further presented an analytical model describing this unusual effect.

More information: Kinnary Patel et al. Dynamics of antipolar distortions, *npj Computational Materials* (2017). DOI:

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