Hidden behaviors of ferroics revealed from multiscale modeling

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Ferroics that undergo structural phase transitions remain in the focus of both scientific and applied research for decades. From fundamental scientific point of view they exhibit perplexing counterintuitive behaviors such as ordering of electric or magnetic dipoles and coupling of these ordering to other stimuli, such as mechanical stress. Consequently, they allow for energy conversion, which makes them top functional materials for many applications, such as sensors, actuators, transistors, memories, to name a few. Often times the origin of their unique behaviors and responses is challenging to reveal owing to the complexity of underlying physics and materials science. Computations often become an excellent tool to resolve the inherent features of these materials. This presentation will showcase some of such recent insights into traditional and emerging ferroelectrics.
One example is the piezoelectric response of hybrid organic-inorganic perovskites. Traditionally such materials exhibit low Curie temperature, polarization and piezoelectric response. We used density functional simulations to reveal the origin of unusually high piezoelectric response in a family of hybrid perovskites [1]. Another example is the dynamics of ferroelectric relaxors that remains the subject of attention and controversy for many years. Atomistic simulations revealed that at high frequency these materials behave as “dynamic” ferroelectrics whose Curie temperature and spontaneous polarization depend on the frequency of applied electric field which could be the key to their hallmark relaxor features [2]. As the last example, we will highlight the success of atomistic simulations in stimulating the progress on the caloric materials.

[1] "Phase switching as the origin of large piezoelectric response in organic-inorganic perovskites: A first-principles-study", P. S. Ghosh, S. Lisenkov, and I. Ponomareva, Phys. Rev. Lett., **125** 207601 (2020). [2] "$Ba(Ti_{1-x},Zr_x)O_3$ relaxors: dynamic ferroelectrics at gigahertz", S. Lisenkov, A. Ladera and I. Ponomareva, Phys. Rev. B , **102** 224109 (2020).

Bio: Inna Ponomareva received her PhD in physics and math from the Institute of Biochemical Physics of Russian Academy of Sciences in 2004. She then joined University of Arkansas for a Postdoctoral work in the area of methodological development and simulations of ferroelectrics. In 2008 she joined faculty in the physics department at the University of South Florida. She has co-authored over 90 research publications, is recipient of NSF CAREER award, and has been promoting computational research through scientific presentations, and various educational and outreach activities.