The Abdus Salam International Centre for Theoretical Physics

College on Multiscale Computational Modeling of Materials for Energy Applications
4 - 15 July 2016

Co-sponsors: INRS Canada, ESF and Psi-k

Combining High-throughput and Spacegroup Techniques to Understand the Microscopic Behaviour of Materials

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Abstract:

Even if ferroelectric materials like $BaTiO_3$ or $KNbO_3$ have been used for decades in a broad range of technological applications, there is still significant debate in the literature concerning their microscopic behavior. For instance, many perovskite materials display a high-temperature cubic phase with zero net polarization, but its microscopic nature is though still unclear, with some materials displaying a very complex energy landscape with multiple local minima. In order to investigate and clarify the microscopic nature of oxide perovskites, we perform a study on a set of about 50 representative ABO_3 systems. We use spacegroup techniques to systematically analyze all possible local displacement patterns that are compatible with a net paraelectric phase, but can provide local non-zero ferroelectric moments. The energetics and the stability of these patterns is then assessed by combining the spacegroup analysis with DFT calculations in a high-throughput fashion, using AiiDA. I will show how we have been able to describe the different classes of microscopic models underlying the perovskite systems using this combined technique. I will

also discuss additional examples from my research, where similar approaches can be adopted for the prediction of the properties of other material systems.