Flexoelectricity

Flexoelectricity in twisted oxide perovskites

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In Short

- Flexoelectricity, an electro-mechanical phenomenon, has recently attracted the attention of researchers as it becomes significant at the nanoscale due to the possibility of extremely large strain gradients
- We employ first-principle calculations to explore the properties of the emerging twisted boundaries.
- Investigate their electronic characteristics, specifically the induced polarization across the resulting screw dislocations.
- Understanding how the flexoelectric response governs the stability and the electronic structure of such boundaries.
- Explore the role of twist angle, nature of materials, and lattice mismatch toward tuning the flexoelectric response.
- Huge super-cells will be considered, imposing the use of parallel calculations.

An unusual electro-mechanical phenomenon, called flexoelectricity, has attracted the attention of researchers in the past few years [1]. Thereby, an electric polarization, is induced by a mechanical strain gradient. Most excitingly, the strength of flexoelectricity is inverse to the sample size and becomes significant at the nanoscale due to the possibility of extremely large strain gradients. For this reason, only recent advancements in synthesis techniques and in control of nanoscale structures, enabled flexoelectricity to become a popular topic in materials science. In contrast to piezoelectricity, flexoelectric coefficients are represented by a fourth-rank polar tensor, *i.e.*, making it an intrinsic and universal property of all dielectric materials and semiconductors, irrespective of the crystal symmetry. As such, flexoelectricity allows for introducing electromechanical functionality in non-piezoelectric materials. Based on the recent significant advances in the experimental setups for measuring the flexoelectric response (2), strong effects have been reported for oxide perovskites.

This project, is devoted to the *ab initio* study of the flexoelectricity in twisted perovskites boundaries.

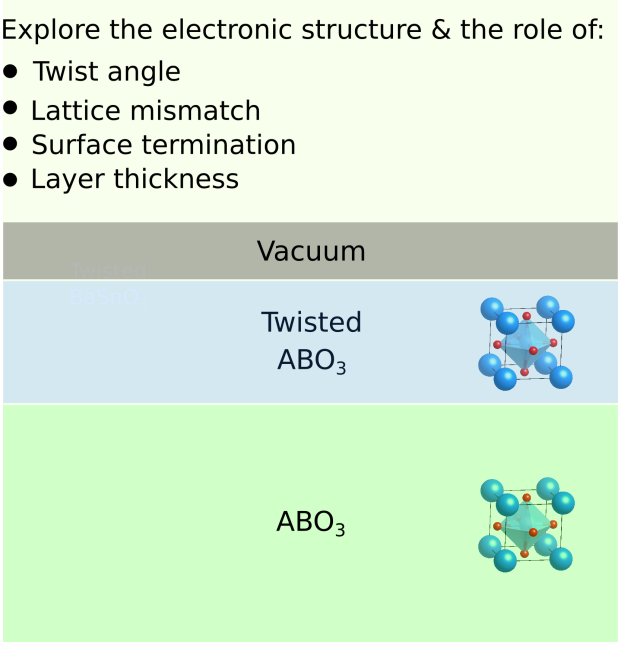

***Figure 1:** Sketch of the different questions we aim to investigate in twisted oxide boundaries.*

We employ density-functional theory (DFT) in order to explore the structural properties, the strain gradient and the induced polarization across the resulting screw dislocation at the boundaries. First, we will optimize the super-cells of twisted layers with different twist angles, surface termination, and layer thickness. Second, we will analyze the strain gradient around the screw dislocation and estimate their polarization which reflects their flexoelectric response. Finally, we will investigate their electronic properties focusing on the formation of two dimensional electron gases. The data obtained from the above studies will be exploited to identify how to tune both the flexoelectric response and the electronic properties.

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https://sol.physik.hu-berlin.de/

More Information

[1] P. Zubko, G. Catalan, A. K. Tagantsev. *Annu. Rev. Mater. Res.* **43**, 387 (2013). doi: 10.1146/annurev-matsci-071312-121634

[2] J. Narvaez, F Vasquez-Sancho, G Catalan. *Nature* **538**, 219 (2016). doi:10.1038/nature19761

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