Ferroelectric perovskites to tune an interfacial two-dimensional electron gas

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In Short

- Heterostructure formed by combining nonpolar $BaSnO_3$ and polar $LaInO_3$ leads to the formation of the two-dimensional electron gas (2DEG) at the interface.
- Tuning the interfacial 2DEG requires precise investigation from both theory and experiment.
- We employ first-principles calculations for understanding the fundamental role of ferroelectrics on the density and distribution of the 2DEG.

The possibility form a two-dimensional electron gas (2DEG) at the interface between two insulating oxide perovskites has attracted tremendous attention in recent years as it is promising for the next-generation of nanoelectronic devices. As such, it is desirable to have the ability to modulate 2DEG properties by an external stimulus. It has been found that ferroelectric materials can be more efficient to control an interfacial 2DEG [1]. Here, we consider a heterostructure formed by combining polar $LaInO_3$ (LIO) and nonpolar $BaSnO_3$ (BSO) perovskites. In this case the polar discontinuity leads to the formation of the 2DEG at the interface within the BSO side.

We focus on the impact of the inclusion of typical ferroelectric perovskites on the density and distribution of the 2DEG. The role of the thickness of the ferroelectric material as well as the amount and direction of its polarization will be investigated. The interfaces are theoretically characterized by *ab initio* approaches. Huge super-cells will be considered, imposing the use of parallel calculations.

This research will be performed hand in hand with our experimental partners.

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https://www.hu-berlin.de/de

More Information

[1] S. I. Kim et al., *Adv. Mater.*, **25**, 4612 (2013). doi:10.1002/adma.201301097

[2] https://fis.hu-berlin.de/converis/portal/Project/402133531?auxfun=&lang=en_GB

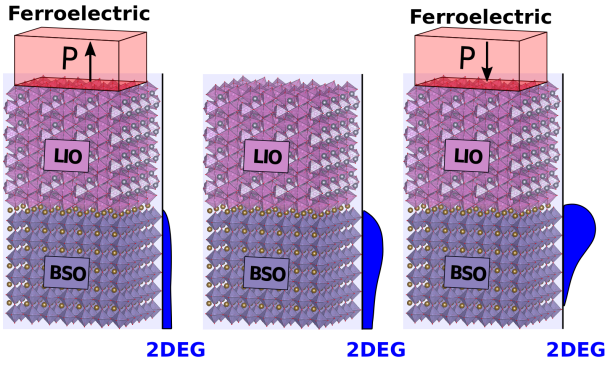

***Figure 1:** Sketch of BSO-based heterostructures and the expected impact of the ferroelectric material on the 2DEG.*

Project Partners

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