Barium stannate based heterostructures for electronic applications

W. Aggoune and C. Draxl, *Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany*

In Short

- For implementation in the electronic devices, barium stannate based heterostructures requires precise knowledge from both theoretical and experimental investigations.
- We employ first-principle calculations for understanding the fundamental physics of the hetero-interfaces.
- Huge super-cells will be considered, imposing the use of parallel calculations.
- This study will be the main key for understanding the physical phenomena is such interfaces.

Perovskite oxides and their heterostructures are emerged to play a key role in the next generation of the electronic devises. The wide tunability of their physical properties spanning insulators, semiconductors, conductors, magnetic and ferroelectric materials are expected to ease and enrich the actual devises such as the ferroelectric gate field-effect transistor (FeFET). For this goal, perovskite barium stannate ($BaSnO_3$), appeared in the last years as the most promising condidates due to its high electron mobility at room temperature, excellent thermal stability, and high transparency [1]. Favourable conduction band offsets with structurally similar oxides such as $SrTiO_3$, $LaAlO_3$, $LaInO_3$, $NaNbO_3$, and many other perovskite oxides are expected to show all their potential in order to develop these applications.

The main goal of this project is to investigate the fundamental physics of $BaSnO_3$ based heterostructures. *Ab-initio* approaches will be applied towards theoretical characterization of perovskite hetero-interfaces. We employ density-functional theory (DFT) and many-body perturbation theory (MBPT) in order to understand the physical phenomena at the interfaces starting from in depth analysis of the intrinsic ground- and excited-states properties of the individual systems. To simulate the interfaces, supercells will be considered, which impose the use of parallel calculations.

To get a deeper insight into the interface structure, the project implies an in-depth understanding of the interface orientation, strain effects, surface terminations, and stability, which will be achieved by optimizing the interface geometries under different conditions. In addition, great focus will lie on the electronic structure of the intrinsic materials and their heterostructures, focusing more on the level alignment at the interface, which is expected to govern the opto-electronic phenomena. This research will be performed hand in hand with our experimental partners at the Leibniz Institute for Crystal Growth (IKZ), the Paul-Drude-Institut für Festkörperelektronik (PDI), and the Technische Universität Berlin (TU).

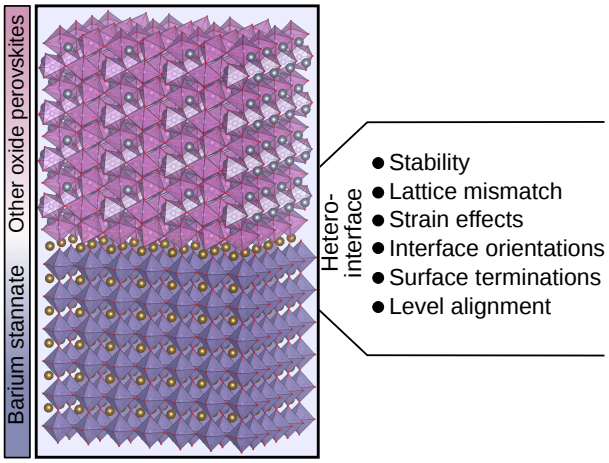

Figure 1: *Sketch of the barium stannate perovskite $BaSnO_3$ heterostructures formed with other similar oxides such as $SrTiO_3$, $LaAlO_3$ and $LaInO_3$. The differences in the intrinsic structural and electronic properties between these materials are expected to govern the resulting interface properties.*

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

More Information

[1] H. J. Kim et al., *Phys. Rev. B,* **86**, 165205 (2012). doi:10.1103/PhysRevB.86.165205

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

Project Partners

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