

## Poster-2-11

**Coupling of octahedra rotations in orthorhombic perovskite heterostructures**

Duncan T.L. Alexander,<sup>1</sup> Hugo Meley,<sup>2</sup> Marcus Schmitt,<sup>3</sup> Bernat Mundet,<sup>1,2</sup> Philippe Ghosez,<sup>3</sup>  
Jean-Marc Triscone,<sup>2</sup> and Stefano Gariglio<sup>2</sup>

<sup>1</sup> *Interdisciplinary Centre for Electron Microscopy (CIME), Ecole Polytechnique Fédérale de Lausanne (EPFL),  
Lausanne, Switzerland*

<sup>2</sup> *DQMP, University of Geneva, 24 Quai E.-Ansermet, CH-1211 Geneva, Switzerland*

<sup>3</sup> *Physique Théorique des Matériaux, Université de Liège (B5), B-4000 Liège, Belgium*

Octahedral rotations patterns in transition metal perovskites affect their physical properties due to the strong coupling between the lattice and the electronic degrees of freedom. Across an interface in an epitaxial heterostructure, the corner sharing of the oxygen octahedra couples the layer-substrate or layer-layer octahedral rotation patterns in competition/together with the epitaxial strain. The consequences and the extent of the rotations imprint are currently at the focus of several studies, since theoretical work indicates that it could be at the origin of novel properties and functionalities.

This work investigates the microscopic details of orthorhombic perovskite heterostructures using X-ray diffraction, scanning transmission electron microscopy and second-principles simulations, revealing that the interface lattice results from a delicate balance between elastic strain energy and rotation modification energy. We observe that the substrate imprints a rotation pattern into thin layers despite the induced elastic strain cost; for thicker films, a transition layer accommodates the change in the rotation pattern between the substrate and the bulk of the layer. We experimentally probe this effect in  $\text{LaVO}_3$  thin films epitaxially grown by pulsed laser deposition onto  $\text{DyScO}_3$  substrates and theoretically confirm this behaviour in  $\text{CaTiO}_3$  structures. This phenomenon opens the way to the control of the orientation of the crystalline axes which often correspond to easy magnetization axes or polarization directions.