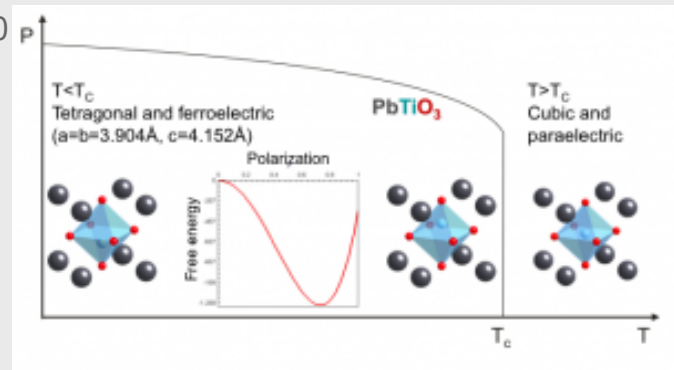


First-Principles Simulations on PbTiO₃/SrTiO₃ Superlattices

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ABSTRACT:

Ferroelectric perovskites are materials of great fundamental and applied interest. This family of materials displays a great range of functionalities, from ferroelectricity to superconductivity. More interestingly, perovskites show a very rich phase diagram allowing for a great tunability playing with doping, epitaxial strain, and the combination of different materials in heterostructures. This has led to the discovery of completely new interface-based phenomena in the last years, for instance a fundamentally new type of ferroelectricity has been discovered in PbTiO₃/SrTiO₃ superlattices, due to the unexpected coupling of ferroelectric and antiferrodistortive structural distortions in these heterostructures [1].

First in this talk, we will present first-principles calculations, within the density functional theory, on the coupling between epitaxial strain, polarization, P , and oxygen octahedra rotations in monodomain (PbTiO₃)_n/(SrTiO₃)_n superlattices [2]. We have studied different periodicities, n ranged from 1 to 3, with an improper ferroelectric behaviour. P is found to be extremely sensitive to strain, and rotates continuously from a c -phase (P oriented along the [001] direction) for compressive strains, to an aa -phase (P along [110]) under tensile strain. The out-of-plane component of P , P_z , is always preserved at the interface to minimize the electrostatic energy, and decreases in the PbTiO₃ layer with respect the bulk value, reflecting the energy cost of polarizing SrTiO₃. At the origin of these new phases with an in-plane component of P , we have found the preference of the polarization in PbTiO₃ to rotate, over an homogeneous decrease of P_z . Around the lattice constant imposed by a SrTiO₃ substrate, the system displays a large piezoelectric response. Changes in polarization are strongly coupled with the response of the oxygen octahedra, whose rotations and tiltings cannot be explained by the usual steric arguments alone. Instead a covalent model on the polarization-tilting coupling is developed.

Second, following the suggestion of a recent experimental work [3], who suggested that the ground state of this system might be actually polydomain for most periodicities, we will also report on simulations on PbTiO₃/SrTiO₃ superlattices including the presence of domains to complement the last experimental results and to better understand the

properties of domain structures in these superlattices.

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[2] P. Aguado-Puente, P. García-Fernández, and Javier Junquera, *Phys. Rev. Lett.* 107, 217601 (2011).

[3] P. Zubko et al. *Phys. Rev. Lett.* 104, 187601 (2010).
