



Canadian Association
of Physicists

Association canadienne
des physiciens et physiciennes

Contribution ID: 3684 Type: **Poster Competition (Graduate Student)** / **Compétition affiches (Étudiant(e) 2e ou 3e cycle)**

(G*) (POS-24) Effect of t_{2g} Orbitals on Ferroelectric Thin Films

Tuesday 20 June 2023 17:34 (2 minutes)

In electron-doped Strontium Titanate (SrTiO₃), ferroelectricity can coexist simultaneously with metallicity. Absent any electrons, the ferroelectric domains will orient themselves into the so-called “Kittel Domains” in order to minimize their free energy. The impact of free electrons on their behaviour remains under active investigation with research suggesting that electron density plays a role in the orientation of the domain walls (e.g. tilt relative to the normal of a thin-film surface). We model a thin-film ferroelectric metal through a self-consistent Landau-Ginzburg-Devonshire free energy, and electron-phonon Hamiltonian. In particular, we consider the coupling of the t_{2g} orbitals with the polarization and their gradients under cubic symmetry, and contrast the behaviour with an uncoupled free electron gas. We are particularly interested in the impact of the electrons on the formation and behaviour of domain walls, and whether they can be tuned to achieve desirable electronic properties (e.g. conductive surfaces or wires) through manipulable characteristics of the material (e.g. film width, external potential, electron density).

Keyword-1

Ferroelectric

Keyword-2

Strontium Titanate

Keyword-3

Electronic Properties

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Session Classification: DCMMP Poster Session & Student Poster Competition (9) | Session d'affiches DPMCM et concours d'affiches étudiantes (9)

Track Classification: Technical Sessions / Sessions techniques: Condensed Matter and Materials Physics / Physique de la matière condensée et matériaux (DCMMP-DPMCM)