Abstract

Ising Spin-Orbit Coupling and Electronic Band Structures of t_{2g} Electrons at Charged Ferroelectric Domain Walls

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The interplay between electron charge, spin, and ferroelectric polarization is under-explored for conducting ferroelectric domain walls.We investigated the electronic band structures of t_{2g} electrons, confined to charged 90° domain walls in barium titanate ($BaTiO_3$), a prototypical perovskite ferroelectric. A key novel aspect of our study is the explicit inclusion of both orbital and spin degrees of freedom in the Hamiltonian. This leads to an Ising-type spin-orbit coupling.We constructed a tight-binding model(TBM) for t_2g electrons that is constrained by symmetries of the domain wall, including time-reversal, mirror, and rotational symmetries. First-principles density functional theory (DFT) calculations were performed to extract the tight binding parameters. Our findings offer new insights into spin-orbit interactions at ferroelectric domain walls and open avenues for their potential use in next-generation electronic and spintronic devices.

Keywords:Ferroelectrics, Charged Domain Walls,2DEG, Symmetries,Spintronics, Spin-Orbit Coupling,Polarization ,Energy Bands,Hamiltonian,Tight-Binding

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