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Possible Flexoelectric Origin of the Lifshitz Transition in Strontium Titanate Interfaces

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Multiple experiments have observed a sharp transition in the band structure of $\text{LaAlO}_3/\text{SrTiO}_3$ (001) interfaces as a function of applied gate voltage. This Lifshitz transition, between a single occupied band at low electron density and multiple occupied bands at high density, is remarkable for its abruptness. In this work, we propose a mechanism by which such a transition might happen. We show via numerical modeling that the simultaneous coupling of the dielectric polarization to the interfacial strain ("electrostrictive coupling") and strain gradient ("flexoelectric coupling") generates a thin polarized layer whose direction reverses at a critical density. The Lifshitz transition occurs concomitantly with the polarization reversal and is first-order at $T = 0$. A secondary Lifshitz transition, in which electrons spread out into semiclassical tails, occurs at a higher density.

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