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POS-F49 – Theory of Hysteretic Behaviour of Doped Quantum Paraelectric-Insulator Interfaces

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Until recently, there has been a general belief that carrier doping destroys spontaneous polarization in ferroelectric materials. However, a small number of materials have been discovered in which ferroelectricity persists into the metallic state. Motivated by this, we study a theoretical model for a MOSFET-like system comprising an insulating polar cap layer and a metallic ferroelectric thin film. We find that adding electrons screens the depolarizing fields and allows for a ferroelectric transition below the insulating film's critical thickness. We show that one may obtain hysteretic behaviour as a function of applied field and that switching the polarization induces a metal-insulator transition at the interface. Depending on the bias voltage, we find both "low-polarization" and "high-polarization" states, similar to what is obtained in insulating ferroelectrics. Our most surprising finding is that the low-polarization state, which has a nearly vanishing average polarization, comprises two domains with large and opposite polarizations, separated by a conducting domain wall. The high-polarization state, on the other hand, contains no such domains. In this case the local polarization is determined by the electron density, where the electrons are confined to either the interface or the back wall depending on the polarization. In both low- and high-polarization states the free charge compensates for the bound charge in the film, making the interior electrically neutral.

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