First-Principles Modeling of Field Effects at Metal-Oxide Heterojunctions

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When the thickness of an oxide film is reduced to few unit cells, its dielectric properties (which are relevant, e.g., for nonvolatile ferroelectric memories and as gate oxides in MOSFET transistors) start to deviate from those predicted by macroscopic models, and crucially depend on the atomic and electronic structure of the interfaces. One particularly important issue is the "dielectric dead layer", which plagues the performance of thin-film perovskite capacitors by substantially reducing the effective permittivity (κ) of the active high-κ material. The microscopic origins of this reduced permittivity, and in particular whether it stems from defects or from the fundamental properties of an ideal metal/insulator junction, are not well understood.

To address this problem from first principles, we will first show how the macroscopic polarization (and the coupling to an external field) can be rigorously defined for a periodic metal-insulator heterostructure [1], by using techniques and ideas borrowed from Wannier-function theory [2]. We will then demonstrate our new method by calculating the dielectric properties of realistic $SrRuO_3/SrTiO_3/SrRuO_3$ nanocapacitors [3]. Building on these ideas, we will finally present two recent applications of our finite-field method: i) critical thickness for monodomain ferroelectricity, and ii) carrier-mediated magnetoelectric effects at the interface between a dielectric and a metallic ferromagnet.

[1] M. Stengel and N. A. Spaldin, accepted in Phys. Rev. B, cond-mat/0511042.

[2] M. Stengel and N. A. Spaldin, Phys. Rev. B **73**, 075121 (2006).

[3] M. Stengel and N. A. Spaldin, Nature (London) **443**, 679 (2006).