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Macroscopic electrostatics at the nanoscale: From ferroelectric capacitors to confined electron gases

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Complex oxides are characterized by a multitude of coupled electronic and lattice degrees of freedom, and therefore constitute an unusually rich playground for experimentalists and theoreticians alike. These microscopic variables manifest themselves in macroscopically measurable quantities such as polarization, magnetization and strain, whose mutual coupling is sought after for applications in multifunctional electronic devices. To understand the interplay of these many factors, density functional theory (DFT) has proven an invaluable tool. However, the treatment of the macroscopic electrical variables (electric fields and polarization), which are a crucial ingredient in describing the experimentally observed response properties, has traditionally been difficult within first-principles calculations. In this talk I will first review a number of recent methodological developments that removed this limitation, thus extending the scopes of first-principles theory to the simulation of realistic devices within arbitrary electrical boundary conditions. Next, I will discuss the evolution of the band offset at a metal/ferroelectric interface as a function of polarization, and its implications for the electrical properties of nanocapacitors. Finally, I will show that, depending on the polarization of the film, a problematic regime might occur where the metallic carriers populate the energy bands of the insulator, making it metallic. As the most common approximations of density functional theory are affected by a systematic underestimation of the fundamental band gap of insulators, this scenario is likely to be an artifact of the simulation. I will discuss a number of criteria to systematically identify this situation in simulations, and effective modeling strategies to describe this peculiar charge compensation mechanism.