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Interface electrostatics in ferroelectric capacitors from first principles

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Capacitors based on ferroelectric perovskites are potentially attractive for applications in nanoelectronics, such as non-volatile random-access memories and high-permittivity gate dielectrics. Thin-film geometries are sought after for optimal efficiency and information storage density. However, in such a regime, strong size effects arise that generally deteriorate the overall performance of the device. Understanding the properties of the oxide/electrode interface is crucial to overcoming these deleterious effects. In this talk I will present our recently-developed methodologies for working at fixed electric displacement field in first-principles density-functional calculations. I will show that application of fixed-D methods to ferroelectric capacitors provides enhanced flexibility for the study of interface-specific issues. I will demonstrate this technique by presenting results for a range of systems based on $PbTiO_3$ or $BaTiO_3$ as ferroelectric, and Pt or $SrRuO_3$ as electrode. Based on a microscopic analysis of interface bonding and electrostatics, I will discuss possible routes to the realization of devices that are free from size effects.