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First principles calculations at fixed dielectric displacement MASSIMILIANO STENGEL, UCSB, DAVID VANDERBILT, Rutgers University, NICOLA SPALDIN, UCSB — With the experimental advances in growth and characterization of superlattices and thin-film capacitors based on ferroelectric perovskites, it is becoming more and more crucial to achieve a fundamental understanding of these structures by accurate first-principles modeling. Unfortunately, difficulties in the treatment of finite electric fields and macroscopic polarization in periodic systems - in particular when metallic electrodes are present - make the application of *ab-initio* techniques to such systems particularly challenging. To address these issues, we present here a method to perform first-principles calculations of periodic systems at a fixed value of the macroscopic dielectric displacement. This technique, which complements previously established strategies to fix P or $\mathcal{E}$, provides a simple and natural way to explore the phase diagram of a ferroelectric system as a function of a single electrical order parameter. We demonstrate the power of our approach by computing the electrical equations of state for two symmetrical ferroelectric capacitors which are based on the same combination of materials, Au and $BaZrO_3$, but are characterized by inequivalent interface geometries and stoichiometries. In particular, we use the information extracted from the centrosymmetric systems to accurately predict the electrical equation of state for an asymmetric capacitor of analogous composition.

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