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*Ab-initio* theory of nanoscale capacitors at finite bias  
MASSIMILIANO STENGEL, Materials Department, University of California, Santa Barbara, NICOLA SPALDIN — We present a novel technique for calculating the properties of an electric field applied to a periodic heterostructure with alternating metallic and insulating layers. This scheme allows us to investigate fully from first- principles the microscopic properties of a thin-film capacitor at finite bias potential. We demonstrate how the capacitance and local permittivity profiles can be readily obtained by performing calculations for the Ag(100)/MgO(100) and SrTiO<sub>3</sub>(100)/SrRuO<sub>3</sub>(100) systems. Applications range from the emerging field of electronic devices based on ferroelectric materials, to the *ab-initio* simulation of electrochemical cells.

Prefer Oral Session  
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