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$_3$(100)/SrRuO$_3$(100) systems. Applications range from the emerging field of electronic devices based on ferroelectric materials, to the ab-initio simulation of electrochemical cells.

Massimiliano Stengel
Materials Department, University of California, Santa Barbara

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