Ab-initio **theory of nanoscale capacitors at finite bias** MASSIMIL-
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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 demon-
strate 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.

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