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Effects of surface layer composition in stabilizing thin film ferroelectrics ALEXIE KOLPAK, University of Pennsylvania, ANDREW RAPPE, University of Pennsylvania — Using first-principles density functional theory calculations, we explore the ramifications of chemically altering the properties of the metal/ferroelectric interfaces in thin film ferroelectric capacitors. We show that a 3 unit-cell-thick $BaTiO_3$ film with $SrRuO_3$ electrodes has a stable, bulk-like polarization when the surface BaO layers are replaced with PbO, in contrast to the unmodified $SrRuO_3/BaTiO_3$ film which only begins to support a small polarization at 8-unit cell thickness. At the other extreme, BaO surface layers completely suppress polarization in $PbTiO_3$ films even with Pt electrodes, which have been shown to stabilize a large bulk-like polarization in unaltered one unit-cell-thick $PbTiO_3$ films. Our results show that in addition to screening by the metal electrodes, the atomic structure and the work functions of the ferroelectric surface layers play key roles in determining stability. Furthermore, our work suggests that particular properties can be achieved in ferroelectric thin films through a combination of chemical surface modification and judicious choice of ferroelectric and electrode materials.

Alexie Kolpak
University of Pennsylvania

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