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Atomic-scale compensation phenomena at ferroelectric interfaces

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The electrical polarization in ferroelectrics induces electrical charges at the surfaces or interfaces of ferroelectric films. The interfacial screening charge at the ferroelectric/electrode interface is now recognized as the most important factor in determining the stability of ferroelectricity in thin films. By combination of first-principles density-functional theory (DFT) calculations and electron microscopy imaging techniques, we investigate the atomic-scale compensation mechanism at the $PbTiO_3/SrRuO_3$ (PTO/SRO) and the $PbTiO_3/SrTiO_3$ (PTO/STO) interfaces. Two very different interfacial reactions to screen the depolarization field are identified. In the case of PTO/SRO, screening by ionic displacement is observed, in addition to electronic screening in the metallic SRO. In the case of PTO/STO, a compensation mechanism by oxygen vacancies is identified. This mechanism is an important option for the design and growth of ferroelectric thin films.

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