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Interfacial Intermixing in Ferroelectric Superlattices from First Principles VALENTINO R. COOPER, Rutgers University, KAREN JOHNSTON, Helsinki University of Technology, KARIN M. RABE, Rutgers University — Ferroelectric superlattices present a unique foundation for creating novel materials for modern devices. In ideal superlattices with perfectly flat, compositionally abrupt interfaces, first- principles studies have shown how factors such as strain due to lattice mismatches, charge compensation and bonding at the interface can be controlled to enhance the ferroelectric properties of the superlattice. In real superlattices, the presence of an additional factor, cation intermixing at the interface, is suggested by high-resolution COBRA studies[1]. As the period of a superlattice decreases, the effect of this intermixing would be expected to become increasingly important. Here, we present results of a first-principles study of the effect of interfacial intermixing on short-period $x_{\mathrm{PT}}/y_{\mathrm{ST}}$ superlattices. We find that the effect of intermixing on the superlattice polarization can indeed be substantial, and use first-principles information about atomic and electronic properties to interpret and model the effect. Implications for other superlattice combinations and experiments will be discussed.

[1]D. D. Fong et al. PRB **71**, 144112 (2005)

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