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Theoretical proposal and investigation of ferroelectric superlattices incorporating head-to-head and tail-to-tail 180° domain walls XIFAN WU, DAVID VANDERBILT, Department of Physics and Astronomy Rutgers, The State University of New Jersey, NJ 08854-8019, USA — In ferroelectric superlattice structures, it is normally assumed that interfaces and ferroelectric domain walls obey electrical boundary conditions involving the matching, or near matching, of the normal component of the electrical polarization across the interface. If this requirement is not met, the interface would normally be metallic, or charged, or both, leading to structures that tend to be unstable. However, the recent development of techniques for atomic-layer epitaxial growth of ferroelectric perovskites opens a novel possibility of synthesizing superlattice structures in which doping layers are intentionally inserted to compensate the polarization charges at the interfaces. For example, using first-principles density-functional methods, we investigate $PbTiO_3$ superlattices in which the polarization alternates from up to down *along the growth direction*, and in which the large polarization charges at the 180° head-to-head and tail-to-tail domain walls are compensated by heterovalent substitution (e.g., Sc or Nb substituting all Ti atoms in one layer). We show that it is theoretically possible to construct insulating superlattice structures of this kind, and investigate their novel properties.

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