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Polarization Dependent Reconstructions of Ferroelectric Surfaces[1] JOHN MARK MARTIREZ, The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania, WISSAM AL-SAIDI, Department of Chemical and Petroleum Engineering, University of Pittsburgh, ANDREW RAPPE, The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania — We present an *ab initio* density-functional study of the surface structures and the thermodynamic stability of ferroelectric tetragonal (001)-oriented slabs of $BaTiO_3$ and $PbTiO_3$, including both cases where the bulk polarization is directed towards (positive) and away (negative) from the surface. We analyzed systematically the total energies of surfaces with different reconstruction symmetries and stoichiometries. The thermodynamic stability diagrams show that the stable surface compositions for the positive and negative surfaces are different, which are in turn different from those of the paraelectric phase. We show that the prevalence of certain surface reconstructions can be understood in the light of the ability of ions to passivate ferroelectric surface charges.

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