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Understanding the surface reconstruction during chemical switching of ultrathin $PbTiO_3$ films from density functional theory[1] JUN HE, BRIAN STEPHENSON, SERGE NAKHMANSON, Argonne National Laboratory — First-principles calculations are used to understand the structure and energetics of the newly discovered 4×1 surface reconstruction that forms under reducing conditions during chemical switching of the ferroelectric polarization in ultrathin films of $PbTiO_3$ with $SrRuO_3$ bottom electrodes coherently strained to $SrTiO_3$ (001). Relaxed surface structures are obtained for polar films with various oxygen stoichiometries in the outermost PbO layer. To model the behavior of many-unit-cell thick films, which are observed to have polarizations near the bulk value, the lowest unit cell(s) of the $PbTiO_3$ film are forced to be polar. The observed surface reconstructions are compared with experimental synchrotron x-ray measurements.

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