Abstract Submitted
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First-principles studies of ultrathin ferroelectric capacitors with Ru-based perovskite electrodes[1] JUN HE, SERGE NAKHMANSON, Materials Science Division, Argonne National Laboratory — First-principles calculations are used to investigate the electrostatics and polarization screening effects in ultrathin $PbTiO_3$ films capped with $SrRuO_3$ or $CaRuO_3$ electrodes under short-circuit boundary conditions. In accordance with previous results, we find that the $SrRuO_3/PbTiO_3/SrRuO_3$ system without antiferrodistortive octahedral rotations is "non-pathological" with respect to the metal/ferroelectric band alignment across the interface. Such rotations, however, have to be explicitly considered to correctly determine the band alignment and polarization screening in the $SrRuO_3/PbTiO_3/SrRuO_3$nanocapacitor. (*) Present address: Vanderbilt University, Nashville, Tennessee 37235 and Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831

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