

Abstract Submitted
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Understanding polarization bias in PbTiO₃/SrTiO₃ and PbTiO₃/SrRuO₃ superlattices SIMON DIVILOV, Stony Brook University, MARIVI FERNANDEZ-SERRA COLLABORATION, GREG HSING COLLABORATION, MATTHEW DAWBER COLLABORATION — We use first principles density functional theory to explain how Pb-O divacancies (DV) and other symmetry breaking factors create a preferred polarization state leading to a bias as seen in experiments. Our results for PbTiO₃/SrTiO₃ (PTO/STO) indicate that Pb-O DV prefer to form on one side of the interface than the other during growth, leading to a preferred polarization state. For PbTiO₃/SrRuO₃ (PTO/SRO) the situation is more complicated due to intrinsic compositional inversion symmetry breaking, which competes with the tendency of DV to form at different sites within the superlattice structure.

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