Polarization
in asymmetrical intermixed interfaces in SrTiO$_3$/PbTiO$_3$ superlattices
SIMON DIVILOV, MARIVI FERNANDEZ-SERRA, GREG HSING, MATTHEW DAWBER, State Univ of NY- Stony Brook — We used first principles density functional theory to study the effects on polarization of asymmetrical intermixing. In our systems, one interface has intermixed A-cations and the other one is pure. We analyze both monodomain and polydomain SrTiO$_3$/PbTiO$_3$ (STO/PTO) superlattices with varying periods. We report how the difference in energy and spontaneous polarization, between the two stable polarization states, scales with period, domain size, thickness of the intermixed layer and oxygen vacancies. Our results are used to explain the origin of the intrinsic polarization asymmetry observed in experimental measurements of ferroelectric hysteresis loops.

Simon Divilov
State Univ of NY- Stony Brook

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