

Abstract Submitted  
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**Polarization**

**in asymmetrical intermixed interfaces in SrTiO<sub>3</sub>/PbTiO<sub>3</sub> superlattices**  
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DAWBER, State Univ of NY- Stony Brook — We used first principles density func-  
tional 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<sub>3</sub>/PbTiO<sub>3</sub> (STO/PTO) superlat-  
tices 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.

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