Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

First-principles study to identify heterostructures of (Pb, Sr)TiO_3 with enhanced ferroelectric polarisation ZHE LIU, Department of Mechanical Engineering, Monash University, Australia — A first-principle cluster expansion method is employed to study the ferroelectric (FE) polarisation properties of $Pb_xSr_{1-x}TiO_3$ perovskite oxide grown on $SrTiO_3$ (001)-substrate. Our results indicate that some heterostructures can significantly enhance polarisation in comparison with the (001) superlattice and the random alloy structures. At $x = 0.5$, an (110) A/B mono-layer superlattice is identified as the structure with the most enhanced polarisation, and at $x = 0.25$, the optimal structure is determined to be a body-centred superstructure. Detailed structural analysis reveals the atomic configurational patterns in the (001) plane that benefit the off-centering of Pb and Sr cations. Explanation is provided in terms of dipole interactions. Our results should apply to other multicomponent FE perovskites as well and they could have a significant impact in the design of FE materials.

Zhe Liu
Department of Mechanical Engineering, Monash University, Australia

Date submitted: 19 Nov 2010 Electronic form version 1.4