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First principles study of the structure and properties of lead indium niobate and its effect on relaxor based materials EAMONN MURRAY, DAVID VANDERBILT, Rutgers University — Recent advanced in the growth of single crystals of relaxor based materials have shown that when $Pb(In_{1/2}Nb_{1/2})O_3$ (PIN) is alloyed into $Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ (PMN-PT) it significantly improves both the depoling temperature and coercive field,[1] overcoming the major drawbacks of these types of systems when compared to PZT. For example, PIN-PMN-PT at a composition of 24/44/32 was shown to have a coercive field more than double that of PMN-PT.[2] Using first-principles methods, we investigate and compare properties of highly ordered PIN systems to allow us to gain some insight into the role of PIN in changing the properties of relaxor-system crystals. This includes an analysis of the most energetically favorable structure and ordering based on the most ordered PIN structures and their possible distortions. Our calculations show that the most stable ordering involves a rocksalt arrangement of the B-site cations. We have also calculated the polarizations, Born effective charges and piezoelectric constants of these structures. The work represents a step towards a more complete understanding of these relaxor-based systems.

[1]G. Hu *et al*, Appl. Phys. Lett. **90**, 032901, (2007)
[2]J. Tian *et al*, Appl. Phys. Lett. **91**, 222903 (2007)

Eamonn Murray
Rutgers University

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