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Crystal Chemistry and Symmetry based approaches to multiferroics.

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The area of improper ferroelectrics and potentially multiferroics has recently received significant attention do the prediction that a combination of a−a−c+ tilting and layered ordering of the A site cations along [001]perov in perovskite ABX3 systems or in the even n Ruddlesden Popper (RP) phases (An+1BnX3n+1), leads to non-centrosymmetric structures which are predicted to have significant switchable polarisations. Two practical examples will be discussed: (i) Suitable doping of the RP phase SrLn2Fe2O7 can induce a polar tilted ground state where weak ferromagnetism and magnetocelecricity are induced by the appearance of the polar tilted state. The transition temperatures and phase sucession is dependant on the degree of doping. (ii) The oxide heterostructure [(YFeO3)5(LaFeO3)5]40,which is magnetically ordered and piezoelectric at room temperature, has been constructed from two weak ferromagnetic AFeO3 perovskites with different A cations using RHEED-monitored pulsed laser deposition.1 Here we elaborate a superspace description of cation ordering in tilted perovskites that allows the prediction of the symmetry of arbitrary cation ordered superlattices, along <100>perov, <110>perov and <111>perov and ordering of both A and B cations, of the various tilted perovskites, which also rationalizes the observed domain structures. This approach is expaned to include magnetic symmetry and the potential for finding other suitable structural distortions in non-perovskite systems will be discussed.

[1] *J. Alaria, P. Borisov, M. Dyer, et al. Chem. Sci., 2014, DOI: 10.1039/C3SC53248H*

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