Abstract Submitted
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Prediction of new ferroelectrics and multiferroics HONGJUN XIANG, Fudan Univ — Ferroelectrics, whose spontaneous electric polarization can be switched electrically, are useful for a range of applications, such as memory or sensing devices. However, relatively few naturally occurring materials are ferroelectric. Available theoretical methods for designing new ferroelectrics are usually restricted to high symmetric systems. We have developed a more general computational approach that can be applied to any system, and have used it to identify previously unrecognised classes of ferroelectrics [1]. With this approach, we show that the R-3c perovskite structure can become ferroelectric by substituting half of the B-site cations. $ZnSrO_2$ with a non-perovskite layered structure can also be ferroelectric through the anion substitution. Moreover, our approach can be used to design new multiferroics as illustrated in the case of fluorine substituted $LaMnO_3$. In addition, we predict that two-dimensional P_2O_3 adopt two possible stable ferroelectric structures (P_2O_3-I and P_2O_3-II) as the lowest energy configurations within a given layer thickness. Their electric polarizations are perpendicular and parallel to the lateral plane, respectively. We propose that P_2O_3 could be used in a novel nanoscale multiple-state memory device [2]. References: 1. Ke Xu, Xue-Zeng Lu, and H. J. Xiang, arXiv:1602.07439 (2016) (To be published in npj Quantum Materials). 2. Wei Luo and H. J. Xiang, Angew. Chem. Int. Ed **55**, 8575 (2016).

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