Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Controlling spontaneous symmetry breaking and topological defect duality in multiferroic InMnO3 from ab initio SINEAD GRIFFIN, NICOLA SPALDIN, ETH Zurich — The rare earth hexagonal manganites are of considerable current interest because of the unusual nature of their ferroelectric phase transition that results in the formation of topological defects exhibiting universal scaling laws[1,2]. Here we use first-principles density functional calculations and symmetry analysis to show that the spontaneous symmetry breaking in the related material InMnO3 can be described using dual Mexican-hat-like potentials that in turn explain the nature of the two recently reported low-symmetry structures. Our analysis also allows us to identify the third, previously unobserved structure that is allowed by symmetry to emerge from the high-symmetry prototype, giving a unified picture of the phase transitions and ground states in the multiferroic hexagonal manganites. [1] S.C. Chae et al., Phys. Rev. Lett. 108, 167603 (2012) [2] S.M. Griffin et al., Phys. Rev. X, 2, 041022 (2012)

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Date submitted: 15 Nov 2013 Electronic form version 1.4