Abstract Submitted
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Ferroelectric control of orbital occupancy in manganites[1] HANGHUI CHEN, Department of Physics, Yale University, SOHRAB ISMAIL-BEIGI, Department of Applied Physics, Yale University — Recent successful fabrication of epitaxial and coherent ferroelectric/manganite interfaces makes it possible to dynamically control charge and spin in manganites [1]. We demonstrate with *ab initio* calculations that in this system, *d*-orbital occupancies of the interfacial Mn atom can also be modulated by flipping the ferroelectric polarization (i.e. flippable orbital polarization). The underlying mechanism is the structural distortions of the oxygen octahedron and the Mn atom inside induced by the ferroelectric polarization. The in-plane orbital $d_{x^2-y^2}$ is stablized by rumpling in MnO_2 layers, while the Jahn-Teller distortion ($c/a > 1$) favors the out-of-plane orbital $d_{3z^2-r^2}$. This ferroelectric control of orbital occupancy serves as a new approach separate from strain for engineering orbital orderings in transition metal oxides.

[1] C.A.F.Vaz et al., Phys. Rev. Lett. 104, 127202 (2010)

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