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Engineered phase competition in A-site-ordered manganites $R\mathbf{BaMn_2O_6}$ (R=Y and rare earth elements) from first principles JIANGANG HE, CRAIG J. FENNIE, School of Applied and Engineering Physics, Cornell University — $(A/A')MnO_3$ manganites for which the A-site cations order in layers, e.g., RBaMn$_2$O$_6$ (R=Y and rare earth elements) show higher charge and orbital ordering temperatures as compared with A-site disordered manganites. The degree of MnO_6 octahedra rotation, and therefore the Mn-O-Mn angle and Mn-O bond length, in RBaMn$_2$O$_6$ varies strongly with the ionic size of the rare earth ion. In fact RBaMn$_2$O$_6$ spans from a ferromagnetic metal (R=La) to an A-type antiferromagnetic metal (R=Pr and Nd), to a CE-type charge/orbital-ordered insulator (R=Sm-Y). The tuning of the electronic and magnetic ground states coincides with changes in the rotation patters and structural transitions from tetragonal (R=La-Nd), to orthorhombic (R=Sm-Gd), to monoclinic (R=Tb-Y) as the radius of R decreasing, reflecting the competition among charge, orbital, magnetic, Jahn-Teller, and lattice degrees of freedom. In this talk we present the epitaxial phase diagram calculated from first-principles for these A/A' layered manganites and discuss the possibility of using an electric-field to control the competition among these phases via octahedral rotation induced ferroelectricity.

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