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Magnetic and Orbital Orders Coupled to Negative Thermal Expansion in Mott Insulators, $Ca_2Ru_{1-x}M_xO_4$ (M = 3d transition metal ion)[1] T.F. QI, O.B. KORNETA, L. LI, Center for Advanced Materials, University of Kentucky, JIANGPING HU, Department of Physics, Purdue University, S. PARKIN, G. CAO, Center for Advanced Materials, University of Kentucky — Ca_2RuO_4 is a structurally-driven Mott insulator with a metal-insulator transition at T_{MI} = 357K, followed by a well-separated antiferromagnetic order at T_N = 110 K. Slightly substituting Ru with a 3d transition metal ion M effectively shifts T_{MI} and induces exotic magnetic behavior below T_N. Moreover, M doping for Ru produces negative thermal expansion in $Ca_2Ru_{1-x}M_xO_4$ (M = Cr, Mn, Fe or Cu); the lattice volume expands on cooling with a total volume expansion ratio, $\Delta V/V$, reaching as high as 1%. The onset of the negative thermal expansion closely tracks T_{MI} and T_N, sharply contrasting classic negative thermal expansion that shows no relevance to electronic properties. In addition, the observed negative thermal expansion occurs near room temperature and extends over a wide temperature interval [1, 2]. These findings underscores new physics driven by a complex interplay between orbital, spin and lattice degrees of freedom.

[1] T.F. Qi, O.B. Korneta, S. Parkin, L.E. DeLong, P. Schlottmann and G. Cao, Phys. Rev. Lett. 105 177203 (2010)
[2] T. F. Qi, O. B. Korneta, S. Parkin, Jianping Hu and G. Cao, Phys. Rev. B 85 165143 (2012)

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T. F. Qi
Center for Advanced Materials, University of Kentucky

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