Orbital and spin physics in transition metal oxides studied by *ab initio* calculations

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Orbital degenerate transition-metal oxides quite often display an orbital ordering which has a great effect on their properties. In this talk, I will first show that due to an interplay among the crystal field, electron correlation and spin-orbit coupling, a special orbital occupation takes place in the quasi one-dimensional cobaltates $Ca_3Co_2O_6$ [1] and Ca_3CoMnO_6 [2], and it well accounts for their significant Ising magnetism. Second, I will address a spin-state ordering and a spin blockade in the layered cobaltate $La_{2-x}Sr_xCoO_4$ [3]. Finally I will report on an unusual 4*d* orbital ordering and a resultant spin-singlet formation in the two-dimensional spin=1 ruthenate $La_4Ru_2O_{10}$ [4]. Our results were obtained through the local-spin-density approximation plus Hubbard *U* calculations.

[1] H. Wu *et al*., Phys. Rev. Lett. 95, 186401 (2005).
[2] H. Wu *et al.*, Phys. Rev. Lett. 102, 026404 (2009).
[3] H. Wu and T. Burnus, Phys. Rev. B (Rapid) 80, 081105 (2009).
[4] H. Wu *et al.,* Phys. Rev. Lett. 96, 256402 (2006).