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Energetics of the spin-state transition in LaCoO3: Total energy calculations using DFT+DMFT RAVINDRA NANGUNERI, HYOWON PARK, University of Illinois at Chicago — In this talk, we will present the energetics of the spin-state transition in strongly correlated LaCoO3 by adopting total energy calculations within density functional theory plus dynamical mean field theory (DFT+DMFT). We computed total energy curves as a function of volume for different spin states including low spin (LS), high spin (HS), and 1:1 mixed HS-LS states. We will show that as the volume is expanded, the mixed HS-LS state becomes energetically stable with a reasonable energy gap to the ground-state LS state. The nature of the HS-LS state is a paramagnetic insulator consistent with experiment while the homogeneous HS state is energetically much higher compared to the LS state. To analyze the dynamical fluctuation effect on the energetics, we also computed DFT+U energy curves by adopting the maximally localized Wannier function as correlated orbitals, same as used in DFT+DMFT calculations. The static correlation effect treated in DFT+U overestimates the tendency to higher spin states and the mixed spin state is wrongly predicted to be the ground state. The effect of the Coulomb interaction U, the Hund's coupling J, and the double counting potential on the energetics will be also discussed.

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