Spin, orbital and charge ordering from LDA+U calculations

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Materials with strong Coulomb correlations between d-electrons show many interesting effects due to the spin, charge and orbital degrees of freedom, for example different kinds of orderings. The LDA+U method with its orbital dependent potential can be used for the investigation of such effects where standard LSDA based approaches fail to reproduce experimental results. We demonstrate this on the following applications:

Charge order:	magnetic Fe_3O_4.
Spin order:	calculation of exchange interaction parameters for the vanadates CaV_2O_5, CaV_3O_7, and CaV_4O_9.
Orbital order:	$KCuF_3$, $LaMnO_3$
Charge and orbital order:	$Pr_{0.5}Ca_{0.5}MnO_3$.
Low-spin to high-spin transition:	trivalent Co in $LaCoO_3$