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Density versus spin-density functional in DFT+U and DFT+DMFT[1] HYOWON PARK, University of Illionis at Chicago, ANDREW MILLIS, CHRIS MARIANETTI, Columbia University — The construction of multi-variable effective action theories such as DFT+U and DFT+DMFT requires the choice of a local subspace of correlated orbitals and an additional variable being either the charge density or spin density. This talk examines the differences between using charge-only and spin-dependent exchange-correlation functionals with the aim of providing guidance for constructing more sophisticated beyond-density functional theories. The widely used spin-dependent approximations to the exchange-correlation functional are found to lead to a large and in some cases unphysical effective exchange coupling within the correlated subspace. Additionally, the differences between Wannier and Projector based definitions of the correlated orbitals are examined, and only small differences are found provided that the orbitals are orthonormal and strongly localized. These results are documented in the context of the rare earth nickelates.

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