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Multi-orbital time-dependent spin-density functional theory for strongly correlation systems: Application to Ce and YTiO₃¹
VOLODYMYR TURKOWSKI, SYED ISLAMUDDIN SHAH, TALAT S. RAHMAN, Physics Department, University of Central Florida — We present a methodology for examining the spectral properties and nonequilibrium response of strongly-correlated electron systems within multi-orbital time-dependent spin-density functional theory. The key element of the theory – exchange-correlation (XC) kernel – is derived from dynamical mean-field theory (DMFT) expressions for two-particle susceptibilities and the electron self-energy for the effective Hubbard model. We demonstrate that the appropriate description of strongly-correlated materials requires a non-adiabatic (time non-local) XC kernel, though the spatial locality in general is not necessary. We apply the formalism to study the spectral properties of cerium and YTiO₃, and establish that the method is capable of describing both metallic and insulating systems. In addition, we present results of the nonequilibrium response of YTiO₃ under an applied short laser pulse. In particular, we analyze the role of inter-orbital interactions in the relaxation dynamics of the system.

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