

Abstract Submitted  
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**TDDFT+DMFT analysis of excitations and relaxation dynamics in alpha-Ce<sup>1</sup>** SYED ISLAMUDDIN SHAH, VOLODYMYR TURKOWSKI, TALAT S. RAHMAN, Department of Physics, University of Central Florida — We apply a combination of time-dependent density functional theory and dynamical mean-field theory (TDDFT+DMFT) to study the excitation spectrum and response of bulk alpha-Ce to an external perturbation by a laser pulse. The excitation spectrum is obtained by solving TDDFT Casida equation with the “free electron” spectrum calculated from density functional theory and the exchange-correlation (XC) kernel extracted from the DMFT charge susceptibility. We pay special attention to the complex role of the hybridization of the f- with the s-, p-, and d-electron states in the system spectrum. The nonequilibrium solution of the TDDFT equations shows that the short-lived local moments of f-electrons get suppressed as the hybridization strength between the f- and other orbitals increases. We also calculate the effective scattering times for the scattering of the f-electrons from the s-, p-, and d-states at different values of the local Coulomb repulsion and exchange J parameters from the corresponding expression for the orbital-resolved XC kernel, and analyze how these scattering processes may affect the dynamics of the system relaxation.

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