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TDDFT+DMFT study of the nonequilibrium response in monoclinic VO2[1] JOSE MARIO GALICIA HERNANDEZ, VOLODYMYR TURKOWSKI, TALAT S. RAHMAN, Department of Physics, University of Central Florida — We study the ultrafast response of insulating (monoclinic) vanadium dioxide system by applying a combination of time-dependent density functional theory (TDDFT) and dynamical mean-field theory (DMFT). Following relaxation of the system using DFT, we calculate its spectrum with DMFT which takes into account inherently electron-electron correlation effects. We consider two types of perturbations: a homogeneous ultrafast laser pulse and a local charge injection. The system response is calculated with TDDFT with the nonadiabatic (frequency-dependent) exchange-correlation (XC) kernel obtained from the DMFT charge susceptibility for the effective Hubbard model of VO2 electronic subsystem. We analyze the details of the dynamics of the breakdown of the metal-insulator transition and the relaxation of the system to equilibrium. In particular, in the case of charge injection we establish the time-dependence of the metallic domain size at different values of the local Coulomb repulsion and exchange energy parameters. We demonstrate that the dynamics of the system is significantly affected by time-resolved electron-electron interactions (memory effects) taken into account through the nonadiabatic XC kernel.

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