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Ultrafast electron dynamics in MnO: a non-adiabatic TDDFT+DMFT study[1] SHREE RAM ACHARYA, VOLODYMYR TURKOWSKI, TALAT S. RAHMAN, University of Central Florida — We have examined the ultrafast electron dynamics in the insulating antiferromagnet MnO when perturbed by a laser pulse. To take properly into account the effects of electron correlations, we have used our newly proposed ab initio approach in which we combine the benefits of Time-Dependent Density-Functional Theory and Dynamical Mean-Field Theory (TDDFT+DMFT) [1]: the TDDFT equations are solved by using the exchange correlation potential obtained from the DMFT solution of an effective Hubbard model. Consequent analysis of the excitation spectrum of the system demonstrates the existence of bound excitonic states with rather strong binding energy of order 100meV. Furthermore, details of the ultrafast charge dynamics allowed us to identify the main channels of the charge response, dominated by the inter-orbital d-electron transitions. We find that strong time-resolved electron-electron interactions play an important role in the response of MnO to a short laser pulse. Good agreement of our result with available experimental data [2] attests to the validity of this TDDFT+DMFT method for understanding electron relaxation dynamics in strongly correlated systems such as MnO. [1] S.R. Acharya et al., Computation 4, 34 (2016); [2] J. Nishitani et al., Phys. Stat. Sol. C 13, 113 (2016).

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