Abstract Submitted
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Absorption spectrum and ultrafast response of monolayer and bilayer transition-metal dichalcogenides[1] VOLODYMYR TURKOWSKI, ALFREDO RAMIREZ-TORRES, TALAT S. RAHMAN, Department of Physics, University of Central Florida — We apply a combined time-dependent density functional theory and many-body theory approach to examine the absorption spectrum and nonequilibrium response of monolayer and bilayer MoS2, MoSe2, WS2 and WSe2 systems. In particular, we evaluate the possibility of existence of bound states - excitons and trions in the undoped systems. In a previous work we have already demonstrated [1] that the binding energies of these states in the monolayer systems are large which makes them available for room temperature applications. We analyze the possibility of ultrafast electron-hole separation in bilayer systems through inter-layer hole transfer, and show that such a possibility exists, in agreement with experimental observations. For doped systems we consider the possibility of Mahan excitonic states in monolayers and show that the binding energy for these states is of the order of 10 meV. We perform a detailed analysis of the relaxation of doped monolayers excited by ultrafast laser pulse by taking into account electron-phonon scattering effects, and demonstrate that ultrafast (10-100fs) processes, including luminescence, may be relevant for these materials.

[1] A. Ramirez-Torres, V. Turkowski, and T.S. Rahman, Phys. Rev. B 90, 085419 (2014).

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