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Theoretical ultra-fast spectroscopy in transition metal dichalcogenides ALEJANDRO MOLINA-SANCHEZ, Physics and Materials Science Research Unit, University of Luxembourg, DAVIDE SANGALLI, ANDREA MARINI, ISM-CNR, Monterotondo, Rome, Italy, LUDGER WIRTZ, Physics and Materials Science Research Unit, University of Luxembourg — Semiconducting 2D-materials like the transition metal dichalcogenides (TMDs) MoS_2, $MoSe_2$, WS_2, WSe_2 are promising alternatives to graphene for designing novel opto-electronic devices. The strong spin-orbit interaction along with the breaking of inversion symmetry in single-layer TMDs allow using the valley-index as a new quantum number [1]. The practical use of valley physics depends on the lifetimes of valley-polarized excitons which are affected by scattering at phonons, impurities and by carrier-carrier interactions. The carrier dynamics can be monitored using ultra-fast spectroscopies such as pump-probe experiments. The carrier dynamics is simulated using non-equilibrium Greens function theory in an ab-initio framework. We include carrier relaxation through electron-phonon interaction. We obtain the transient absorption spectra of single-layer TMD and compare our simulations with recent pump-probe experiments [2]. [1] D. Xiao et. al., Phys. Rev. Lett. **108**, 196802 (2012). X. Xu et. al. , Nature Physics **10**, 343 (2014). [2] Y. T. Wang, et. al. , Scientific Reports **5**, 8289 (2015).

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