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].