Ab initio calculation of resonant Raman intensities of transition metal dichalcogenides[1] HENRIQUE MIRANDA, SVEN REICHARDT, ALEJANDRO MOLINA-SANCHEZ, LUDGER WIRTZ, University of Luxembourg — Raman spectroscopy is used to characterize optical and vibrational properties of materials. Its computational simulation is important for the interpretation of experimental results. Two approaches are the bond polarizability model and density functional perturbation theory. However, both are known to not capture resonance effects. These resonances and quantum interference effects are important to correctly reproduce the intensities as a function of laser energy as, e.g., reported for the case of multi-layer $MoTe_2$[1]. We present two fully *ab initio* approaches that overcome this limitation. In the first, we calculate finite difference derivatives of the dielectric susceptibility with the phonon displacements[2]. In the second we calculate electron-light and electron-phonon matrix elements from density functional theory and use them to evaluate expressions for the Raman intensity derived from time-dependent perturbation theory. These expressions are implemented in a computer code that performs the calculations as a post-processing step. We compare both methods and study the case of triple-layer $MoTe_2$. [1] G. Froehlicher et al. Nano Lett. **15,** 6481 (2015) [2] Y. Gillet et al. Phys. Rev. B **88,** 094305 (2013)

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