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Resonant-Raman Intensities of N-layer Transition Metal Dichalcogenides from First Principles HENRIQUE MIRANDA, University of Luxembourg, GUILLAUME FROEHLICHER, ETTIENNE LORCHAT, FRANOIS FERNIQUE, IPCMS (CNRS - Universit de Strasbourg), ALEJANDRO MOLINA-SNCHEZ, University of Luxembourg, STPHANE BERCIAUD, IPCMS (CNRS - Universit de Strasbourg), LUDGER WIRTZ, University of Luxembourg — Transition metal dichalcogenides (TMDs) have interesting optical and electronic properties that make them good candidates for nano-engineering applications. Raman spectroscopy provides information about the vibrational modes and optical spectrum at the same time: when the laser energy is close to an electronic transition, the intensity is increased due to resonance. We investigate these effects combining different ab initio methods: we obtain ground-state and vibrational properties from density functional theory and the optical absorption spectrum using GW corrections and the Bethe-Salpeter equation to account for the excitonic effects which are known to play an important role in TMDs. Using a quasi-static finite differences approach [1], we calculate the dielectric susceptibility for different light polarizations and different phonon modes in order to determine the Raman tensor of TMDs, in particular of multi-layer and bulk $MoTe_2$. We explain recent experimental results for the splitting of high-frequency modes [2] and deviations from the non-resonant Raman model. We also give a brief outlook on possible improvements of the methodology. [1] Y. Gillet et. al., Phys. Rev. B 88, 094305 (2013). [2] G. Froehlicher et. al., Nano Lett. 15, 6481 (2015).

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