

**Montag, 20.11.2017 um 15:15 Uhr**  
**Ort: Seminarraum 87, Wilhelm Klemm-Straße 10**

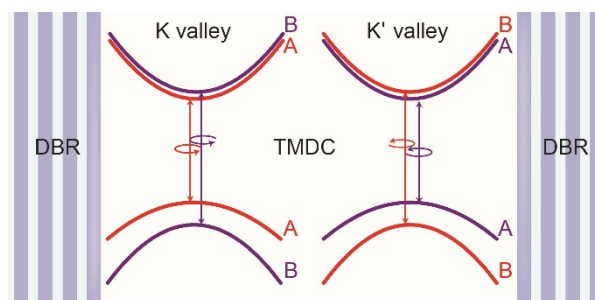
## Microscopic simulation of second harmonic generation in a transition metal dichalcogenide monolayer



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Semiconducting monolayers of transition metal dichalcogenides (TMDCs) show strong optical responses. In the linear regime pronounced exciton lines are visible and in the nonlinear regime a strong second harmonic generation has been observed. By embedding a TMDC monolayer in a photonic structure the optical signals from a TMDC monolayer can be efficiently tailored.

In this talk, I will present a novel method to calculate the linear and nonlinear optical signals of a  $\text{MoS}_2$  monolayer. For the simulation we combine a finite difference time domain (FDTD) method, which accounts for the light field dynamics, and couple it to the semiconductor Bloch equations, which give us a microscopic description of the carrier dynamics in the TMDC monolayer [1]. The strong excitonic effects are taken on board by calculating the Coulomb interaction dynamically on the Hartree-Fock level, while the second harmonic generation is achieved by introducing a permanent dipole. Using our self-consistent method, we determine the shape of the second harmonic signal in a  $\text{MoS}_2$  monolayer and discuss its dependence on the exciting frequency. We show that by an appropriately designed cavity a strong enhancement of the second harmonic can be achieved.



[1] S. Guazzotti, A. Pusch, D. E. Reiter, and O. Hess, Tailoring the optical response of a transition metal dichalcogenide monolayer through photonic structures, to be submitted (2017)