

Aktuelle Fragen der Nanophysik

## Montag, 14.06.2021 um 15:15 Uhr Online Seminar

## Phonon influence on linear optical properties of TMDC monolayers



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Monolayers of transition metal dichalcogenides (TMDCs) hold great promise for excitonic and polaritonic applications due to their huge exciton binding energies and strong exciton-light interaction. Also, the exciton-phonon interaction is particularly strong in these materials and leads to pronounced asymmetric line shapes of optical signals. Therefore, it is of high interest to calculate and understand these phenomena.

In this talk we promote a computationally light method, a time convolutionless master equation (TCL) for the excitonic polarization, to compute linear optical spectra under the influence of strong exciton-phonon interaction. Treating  $MoSe_2$  as an example, we show by comparison to high-order correlation expansion methods that the TCL can describe the spectra very accurately despite its simplicity. In particular, the method reveals the occurrence of asymmetric line shapes in the optical spectra of a TMDC monolayer.

In the next step, we consider a MoSe<sub>2</sub> monolayer within a high-quality microcavity leading to the formation of exciton-photon polaritons. Treating the coupling between polaritons and phonons again by the TCL, we discuss the resulting phonon influence on the line shape. We find a low-energy shoulder of the upper polariton branch due to phonon-assisted processes opposed to the usual high-energy shoulder of the excitonic resonance in the case of a bare monolayer because of the peculiar polariton band structure. Due to the latter, the lower polariton branch is decoupled from acoustic phonons to a large extend. Thereby our results give insight into the exciting interplay of excitons, photons and phonons in TMDC monolayers.

