

PHYSICAL COLLOQUIUM

INVITATION

Monday, 03.12.2018, 4.15 p.m., W2-1-148

speaks

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about

"Theoretical spectroscopy of 2D materials"

Optical and vibrational spectroscopy play a strong role in the characterization and investigation of layered, quasi-2D, materials such as graphene, hexagonal boron nitride (hBN) and transition metal dichalcogenides (TMDCs). In many cases, experimentalists and theoreticians work closely together in order to draw a maximum of information from the position, intensity and width of the peaks in the spectra. We give an overview over the state-of-the-art in ab-initio methods for electronically excited states. In particular, electron-phonon (or, more precisely, exciton-phonon) coupling must be taken into account whenever the vibration of the nuclei plays a role.

We present two recent results on theoretical spectroscopy involving electron-phonon scattering. First, we will present calculations of phonon-assisted indirect absorption/emission in bulk hBN. Despite its very simple atomic structure (4 atoms per unit cell), the optical spectra of this material display a rich spectroscopic signature due to its indirect band gap and the resulting interplay of phonons and excitons. In the second part, we will show examples how time-dependent many-body perturbation theory can help to understand ultra-fast spectroscopy of 2D materials. In particular, we show that electron-phonon coupling is the driving mechanism for the temperature-dependent valley depolarization in time-resolved Kerr rotation spectroscopy of TMDCs.

All interested persons are cordially invited.

Sgd. Dr. Levent Gütay