

NANO COLLOQUIA 2023 - S3 SEMINAR

Exciton-phonon coupling. Theory and modelling from first principles

Thursday March 2, 2023 – 15:00

ON-SITE - S3 Seminar Room, Third Floor, Physics Building

ONLINE - <https://tinyurl.com/FulvioPaleari>

Speaker

Fulvio Paleari - CNR Nano S3

Abstract

The problem of exciton-phonon interaction in crystals concerns the simultaneous description of the coupling of excited electron-hole pairs both between themselves and with lattice vibrations. It has become increasingly relevant to both experimental and theoretical research. It is invoked, for example, to explain fine structures in optical absorption and luminescence spectra of low-dimensional semiconductors, to model the width of excitonic spectral peaks, and to explain the out-of-equilibrium carrier dynamics in ultrafast spectroscopy.

I will first briefly introduce the concepts of phonons and excitons from a many-body point of view and in the context of ab initio, first-principles simulations.

Then, starting from the static Bethe-Salpeter equation (BSE) - which is the state-of-the-art tool to compute excitons - I will present several novel theoretical-computational approaches to exciton-phonon interaction.

The approaches differ theoretically on when the phonon interaction is turned on – either at the excitonic or electronic level – and computationally on the technique employed to obtain the coupling – either via finite-difference derivatives of the excitonic response function, or via a dynamical extension of the BSE. All these approaches are available and/or under development via the Yambo many-body code.

During the discussion I will present relevant applications on the phonon-assisted satellites appearing in the optical spectra of hexagonal boron nitride and on the phonon-mediated exciton scattering amplitudes in monolayer transition metal dichalcogenides. Finally, I will give perspectives for future work on this rich and fascinating topic.

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