Phonon-assisted luminescence in layered materials

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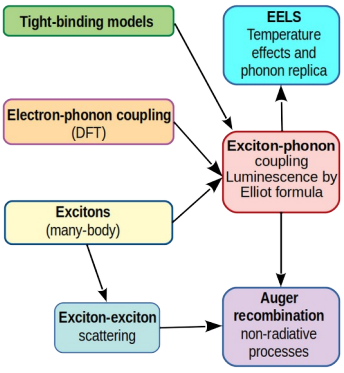
CONTEXT:

In standard solid state physics textbooks direct band gap semiconductors are considered efficient light emitters while indirect ones are regarded as inefficient. Silicon is a typical example: its indirect nature prohibits applications in optoelectronics. This fact has motivated significant research activity to engineer silicon and transform it into a direct gap semiconductor by means of defects, nanostructuring, etc. A more recent and remarkable example of indirect to direct gap transition is represented by MoS_2 nanostructuring. The luminescence signal increases by orders of magnitude passing from multi-layer to single layer MoS_2 with an associated indirect to direct band gap transition.

Hexagonal boron nitride (hBN) seems to defy this rule: it has a large indirect band gap of about 7 eV,but it has recently attracted much attention from the scientific community as a very efficient light emitter in the ultraviolet energy range. An internal quantum yield of about 45% has been reported for hBN, much closer to the 50% one of ZnO (direct band gap) than to the 0.1% one of diamond (indirect band gap)[1]. This goes against the common wisdom that indirect band gap insulators are bad light emitters. Only recently, thanks to accurate and precise measurements and theoretical calculations[2,3], it has been possible to clarify that luminescence is due to phonon assisted transition . This result was further confirmed by measures of isotope effects in luminescence , and the study of excitons dispersion by means of electron-loss spectroscopy[4].

PROJECT:

In this project we want to develop a a new theoretical framework to study exciton-phonon coupling in layered materials. This theoretical framework will allow: 1) an efficient calculation of luminescence spectra mediated by phonons in bulk and 2D materials; 2) the inclusion for the first time of temperature effects and phonon replica in EELS spectra; 3) the evaluation of the exciton Auger recombination that is one of the most important limiting factor for the luminescence.



A schematic representation of the proposed theoretical advances is presented in figure. All these advances will be benchmarked to the measurements performed two experimental groups in Paris and Versailles.

Once developed, this methodology could find application in the study of a large number of physical phenomena as exciton diffusion and relaxation, time-resolved luminescence in two-dimensional crystals or bulk semiconductors.

Keywords: luminescence, electron-phonon coupling, ab-initio, computational physics

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