Phonon assisted luminescence in hexagonal Boron Nitride

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Hexagonal Boron Nitride (hBN) as graphite is a lamellar compound, both have the same honeycomb structure inside a monolayer. They also share many physical properties and they can be exfoliated in monolayers for Van der Waals heterostructures. However a difference does exist, graphite is a gapless compound while hBN is a wide band gap material. In particular first principles calculations agree upon the existence of an indirect quasiparticle band gap : the conduction band minimum sits at the M point while the valence band maximum is around the K point of the Brillouin zone.

On the experimental side the nature of the electronic band structure of hBN has animated a long-standing debate. Pioneering works of Watanabe et al. [1] have revealed the high UV radiative efficiency of hBN at room temperature. He first came to the conclusion that hBN was driven by direct excitonic recombination. Recently Cassabois et al. [2] instead explained the luminescence lines to phonon-assisted recombination from an indirect exciton.

Aiming to describe phonon-assisted luminescence a theoretical formulation that combines electron-hole interactions and electron-phonon coupling is needed. In recent years the method of finite differences [3] turned out to be a powerful tool to treat the electron-phonon coupling in a perturbative way. So we combine Green’s function theory with finite difference electron-phonon coupling to get an accurate description of the phonon assisted luminescence spectrum of hBN.

[1] Watanabe et al. Nature Materials 3, 404 (2004)
[2] Cassabois et al. Nature Photonics, 10, 262 (2016)
[3] B. Monserrat, Journal of Physics: Condensed Matter 30, 083001 (2018)