

# Fine structure of phonon replicas and exciton-phonon interaction in the strong coupling regime in hexagonal boron nitride

T. Q. P. Vuong<sup>\*</sup>, G. Cassabois, P. Valvin, B. Gil

Coulomb, UMR 5221 CNRS-Université de Montpellier, 34095 Montpellier, France

Corresponding author : vuongquynhphuong90@gmail.com

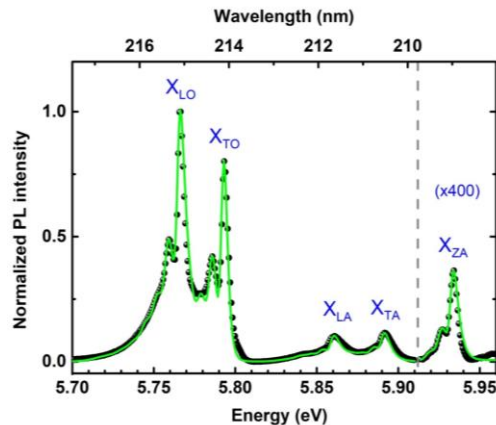
Hexagonal boron nitride (h-BN) is a wide bandgap semiconductor promising for applications in deep UV that raises many interests of scientists in this material. The recently publication of Cassabois *et al.* [1] shows the experimental evidence by photoluminescence (PL) for the indirect bandgap of h-BN, with phonon replicas and an indirect exciton transition in PL spectrum that was confirmed by polarization-resolved PL [2]. In our work, we focus on understanding the intrinsic optical and electronic properties of h-BN in deep ultraviolet which are determined by the lattice vibrations. Firstly, we show that the fine structure of the emission spectrum in h-BN arises from the phonon replicas (at T point) associated with the overtones of the interlayer shear mode (at zone center). We present the excellent agreement of the theoretical fit with the emission spectrum above 5.7 eV (Fig.1), obtained under the convolution of a cumulative Gaussian broadening as a function of overtones index. The only varying parameter is the group velocity for each phonon branch, thus controlling the intrinsic properties of h-BN [3]. Secondly, we prove for the first time that h-BN provides a text-book example for the strong coupling regime of the exciton-phonon interaction due to: (i) The line-shape has a Gaussian profile in contrast to the weak coupling regime with Lorentzian lines and (ii) the linewidth increases as  $\sqrt{T}$  in contrast to the weak coupling regime with a linear increases with temperature following the theoretical predictions of Toyozawa [4].

[1] G. Cassabois et al, Nature Photonics, **10**, 262-266 (2016).

[2] Vuong et al, 2D Materials, **4**, 011004 (2017).

[3] Vuong et al, Physical Review B, **95**, 045207 (2017).

[4] Y. Toyozawa, Progr. Theor. Phys. 20, 53 (1958).



**Figure 1** : Photoluminescence spectrum of h-BN at 8K includes experimental data (symbol) and theoretical fit (green line).