Understanding optical absorption and luminescence in hBN: a tool for a characterisation metrics from bulk to the monolayer

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hBN layers meet a growing interest for deep UV LED [1], and has become a strategic material for the fabrication of van der Waals heterostructures. Stacked with any other 2D material it can reveal the best of their physical properties [2]. However, hBN optoelectronic properties remain much less characterized and understood than other 2D materials.

In this talk, we review recent advances made thanks to the development of appropriate spectroscopies in the UV range - cathodoluminescence (CL) at 4K and Raman [3,4], angular resolved EELS [5] combined with ab initio simulations and tight binding modeling [6]. Thanks to these tools, a h-BN characterization metrics has been developed on the basis of their original optical properties, governed, in the energy range 5.5 – 6 eV, by strong excitonic effects easily trapped at structural or chemical defects [3]. We shall discuss the interplay between structure, defects and spectroscopic properties and how these properties can be further exploited for sample benchmarking [3, 7].

Beyond this effort, the talk will also address the recent advances made for the understanding of the high luminescence observed although bulk hBN is an indirect band gap material [1,8,9]. To that aim, the efficiency of radiative recombinations has been measured on a reference single crystal using temperature - dependent CL and compared to that diamond and ZnO [10]. The luminescence of hBN is confirmed to be unusually high and is found to remain constant from 10 to 300K. Enlighting analysis of this behaviour is provided by ab initio calculations of the exciton dispersion in bulk hBN. First, the lowest-energy exciton (iX) is found at 5.97eV and to be indirect, as expected for an indirect band gap, with a binding energy equal to 300 meV. This dispersion behavior accounts for an assignation of the luminescence to phonon assisted recombinations of the indirect exciton as proposed in [11] and for the assignation of the tiny peak observed in CL spectra at 5.956 eV to the zero-phonon radiative recombination of iX [10]. Further iX high binding energy is consistent with the temperature behavior of the luminescence, the high yield being the signature of a strong exciton phonon coupling. Second, calculations also confirm the direct exciton (dX) with a binding energy of 670 meV [10], an energy which turns to be only 100 meV above the indirect one. It comes out that bulk hBN displays a peculiar behavior where luminescence and optical absorption are due to different excitons, one resonant and one non resonant [10].

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