

Optical properties of h-BN: from bulk to monolayer

C. Elias^{1,8}, G. Fugallo², P. Valvin¹, T. Pelini¹, A. Summerfield³, J. Li⁴, C. l'Hénoret¹, C. J. Mellor³, T. S. Cheng³, L. Eaves³, C. T. Foxon³, P. H. Beton³, F. Sottile⁵, M. Lazzeri⁶, A. Ouerghi⁷, J. H. Edgar⁴, S. V. Novikov³, B. Gil¹ & G. Cassaboïs¹

1. *Laboratoire Charles Coulomb UMR 5221 CNRS-Université de Montpellier, 34095 Montpellier, France*
2. *LTeN UMR 6607 CNRS-PolytechNantes, Université de Nantes, 44306 Nantes, France*
3. *School of Physics and Astronomy, University of Nottingham, Nottingham NG7 2RD, UK*
4. *Tim Taylor Department of Chemical Engineering, Kansas State University, Manhattan, Kansas 66506, USA*
5. *Laboratoire des Solides Irradiés, Ecole Polytechnique, CNRS, CEA/DRF/IRAMIS, Institut Polytechnique de Paris, 91128 Palaiseau, France*
6. *Sorbonne Université, CNRS UMR 7590, MNHN, IMPMC, 75005 Paris, France*
7. *C2N CNRS-Univ Paris Sud, Université Paris-Saclay, 91120 Palaiseau, France*
8. *LuMIn laboratory, ENS Paris-Saclay, campus d'Orsay, Bat 520, Orsay, France*

Hexagonal boron nitride (h-BN) is a 2D material, iso-structural to graphite, with a wide band gap (~6eV). In 2004, h-BN demonstrated its ability to efficiently emit light in the deep ultra-violet (DUV) after the synthesis of high quality h-BN crystals in Japan [1]. The demonstration of lasing at 215 nm make of h-BN one of the most promising materials for DUV optoelectronics. However, its fundamental opto-electronic properties have not been fully understood.

In 2016, two photon-spectroscopy demonstrated that its fundamental exciton is of indirect nature and the resulting recombination process is assisted by phonons along M→K [2]. Nevertheless, there is a direct exciton at the K point with an energy slightly above the fundamental one. The interplay between the indirect and direct excitons in bulk h-BN was not fully understood because reflectivity and absorption experiments have been very limited in hBN. During this talk, I will present reflectivity measurements performed on bulk h-BN crystals at cryogenic temperatures and for an energy range between 5.5 eV and 7 eV. These results show the contribution of the indirect and direct excitons to the absorption process of bulk h-BN and reveal the effect of electronic flat bands to its optical response [3].

In h-BN, like in other 2D materials, when reducing the dimensionality from a 3D system (bulk) to a 2D system (monolayer), the nature of the gap changes. The calculations show a change from an indirect gap (bulk) to a direct gap (monolayer). This indirect-direct gap transition has never been observed in h-BN, and consequently the opto-electronic properties of the monolayer have never been studied experimentally. During this presentation, I will show the first experimental evidence of a direct gap transition in monolayer h-BN by presenting photoluminescence and reflectivity measurements performed on BN monolayer (mBN) grown by Molecular Beam Epitaxy (MBE) at high temperature on graphite substrates. Our results demonstrate for the first time the presence of an optical transition at 6.1 eV associated to the direct gap in mBN [4].

References

- [1] Watanabe et al., Nat. Mat. 3, 1134 (2004)
- [2] G. Cassaboïs et al., Nature Photonics, 10, 262-266 (2016)
- [3] C. Elias et al., PRL, **127**, 137401, 2021
- [4] C. Elias et al., Nature Communications, 10 (1), 2639,2019