Excitonic properties in layered Boron Nitride and BN/BN homostructures: a Review

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Despite its simple crystal structure, layered boron nitride features a surprisingly complex variety of phonon-assisted luminescence peaks. This talk will review main achievements on the study of excitonic properties performed thanks to a time resolved (TRCL) system dedicated in the UV range combined with first-principles computational techniques.

First, we solved a problem that had been misunderstood for 20 years, namely the unusually high luminescence efficiency of hexagonal boron nitride bulk crystals despite the indirect band gap of this material. Thanks to TRCL experiments, we have provided a first estimate at 27 ns of the radiative life time of free excitons emitting at 215 nm from a single experiment comparing hexagonal BN crystals issued from different synthesis routes. This was done by measuring, for each sample, both the internal quantum yield and the exciton life time. The estimate is much shorter than in other indirect bandgap semiconductors, that we explain by the compacity of the exciton complex and also by the small difference in energy between direct and direct excitons [1, 2].

Second, we compared UV-light emission in hexagonal and rhombohedral bulk BN crystals, which differ in the way the layers are stacked. We show that observed differences between the two polytypes are qualitatively and quantitatively explained using a fully first-principles computational technique that takes into account radiative emission from "indirect," finite-momentum excitons via coupling to finite-momentum phonons [3].

Third, we have studied the excitonic luminescence arising at 4 eV at the interface between two disoriented BN flakes, following a deterministic approach for elucidating the interplay between twist angles, defects and excitons. The exciton properties were investigated by exploring their luminescence dynamics in TRCL as a function of twist angle and temperature in a set of exfoliated crystals from different BN sources whose thickness was optimized in order to favor the exciton diffusion towards the interface between the flakes [4]. From the analysis of our sample set, we propose that the 4-eV emission originates from a self-trapping mechanism of the exciton at the twisted interface, which consists in a local distortion of the lattice around the site on which the exciton has trapped itself [5].

References

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