MS-2-O-1827 Nanometric resolved cathodoluminescence on few layers h-BN flakes

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Within the latest years number of layered materials at reduced dimensions have demonstrated remarkable optical properties. However most studies focused on perfect system and the role of defects as optical active centers remain unexplored. Hexagonal boron nitride(h-BN) is one of the most promising candidates for light emitting devices in the far UV, presenting a single strong excitonic emission at 5.8 eV. However, a single line appears only in pure monocrystals, obtained through complex process[1]. Common h-BN samples present more complex emission spectra that have been attributed to the presence of structural defects. Despite a large number of experimental studies up to now it was not possible to attribute specific emission features to well identify defective structures.

Here we address this fundamental questions by adopting a theoretical and experimental approach combining few nanometer resolved Cathodoluminescence (CL) techniques with high resolution TEM images and state of the art quantum mechanical simulations.

Recently, the Orsay team has developed a CL detection system integrated within a STEM[2]. This unique experimental set up is now able to provide full emission spectra with a resolution as low as few tens of meV associated with an electron probe size of 1nm. A CL spectrum-image can thus be recorded in parallel with an HAADF image.Nanometric resolved CL on few-layer chemically exfoliated h-BN crystals have shown that emission spectra are inhomogeneous within individual flakes. Emission peaks close to the free exciton appear in extended regions. Complementary investigations through high resolution TEM allow to associate these emission lines with extended crystal deformation such as stacking faults and folds of the planes[3]. By means of ab-initio calculations in the framework of Many Body Perturbation Theory (GW+BSE) we provide an in-depth description of the electronic structure and spectroscopic response of bulk hexagonal boron nitride in the presence of extended morphological modifications. In particular we show that, in a good agreement with the experimental results, additional excitons are associated to local symmetry changes occurring at crystal stacking faults.

Additional features appearing within the band gap present a high spatial localization, typically less than 100 nm, and thus they can be related to individual point defects. When addressed individually through a highly focused electron probe they might have a single photon emitter quantum character. This hypothesis has been recently confirmed by experiments combining our CL system with an Hanbury Brown and Twiss interferometer.

Fig. 1: a Bright field and b dark field images of an individual BN flake. c Overall emission spectrum of the flake and individual spectra taken at specific probe positions indicated in panel b. d-h Emission maps for individual emission peak. Intensity is normalized independently within each individual map.