Gate-tunable light-emitting device made of defective boron nitride nanotubes: from ultraviolet to the visible

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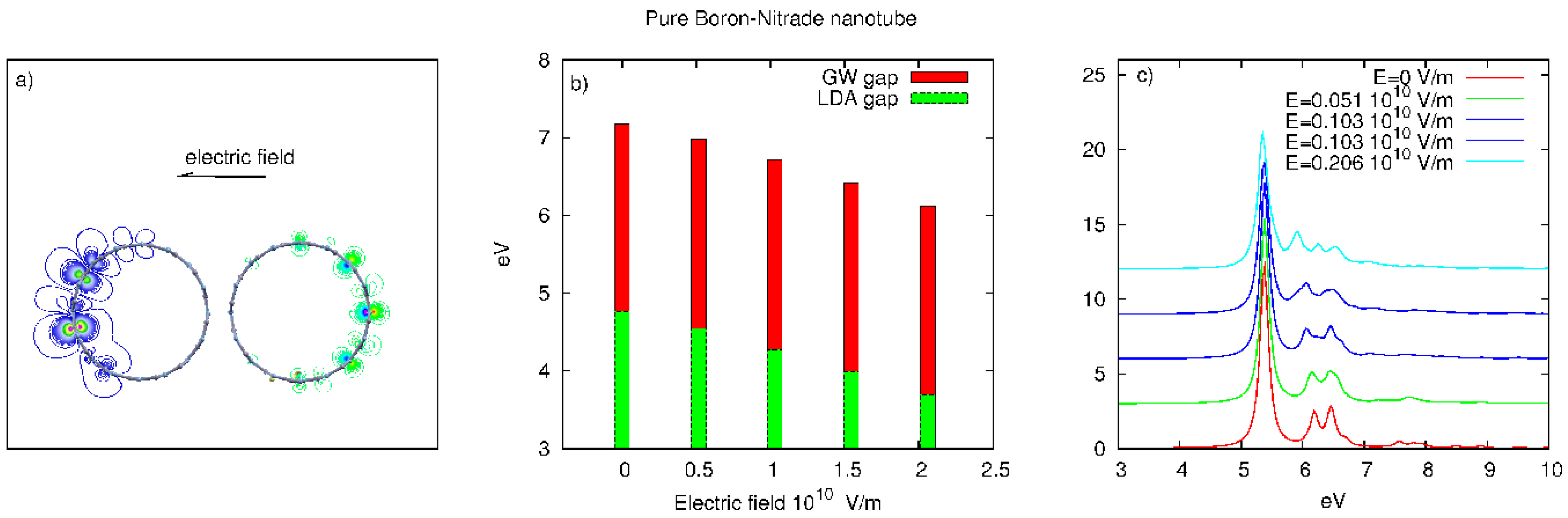
Boron nitride nanotubes (BNNTs) are one-dimensional(1D) systems, with diameters of few nanometers. They possess a large band gap regardless of chirality or diameter. This property has been already employed to produce light emitting devices in the ultra-violet range. Here we show that introducing particular defects in BNNTs it is possible to obtain light emission in the visible range with a tunable frequency by mean of an external transverse electric field.

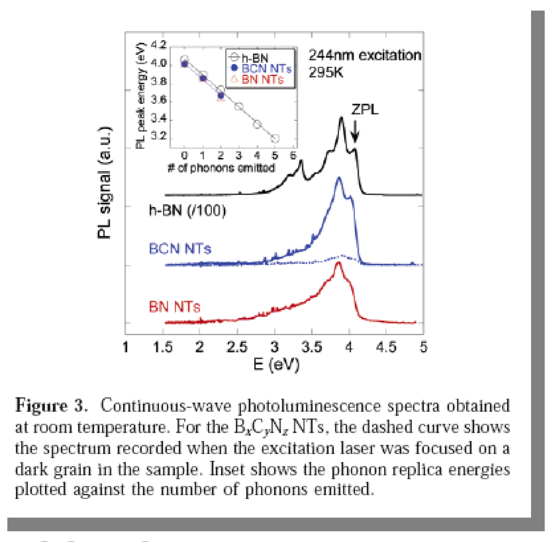
Pure BN nanotubes within an external electric field

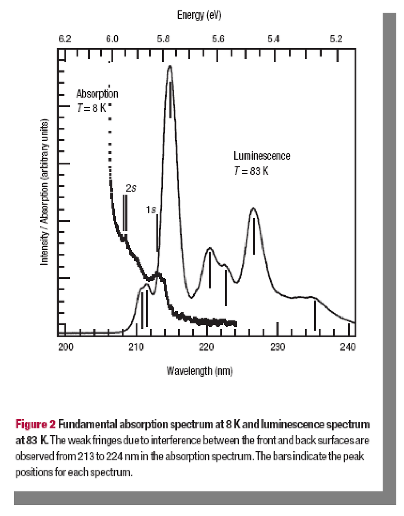
A transverse electric field **shrinks the gap of pure BNNTs** as shown in panel b). Surprisingly the gap shrinking does not affect the optical properties. **The main exciton remains in the same energy position**, while a small fraction of its spectral weight is redistributed to higher excitons, see panel c). This is due to the fact that the conduction and valence orbitals contributing to the gap reduction are localized on the opposite side of the tube, having therefore zero overlap.



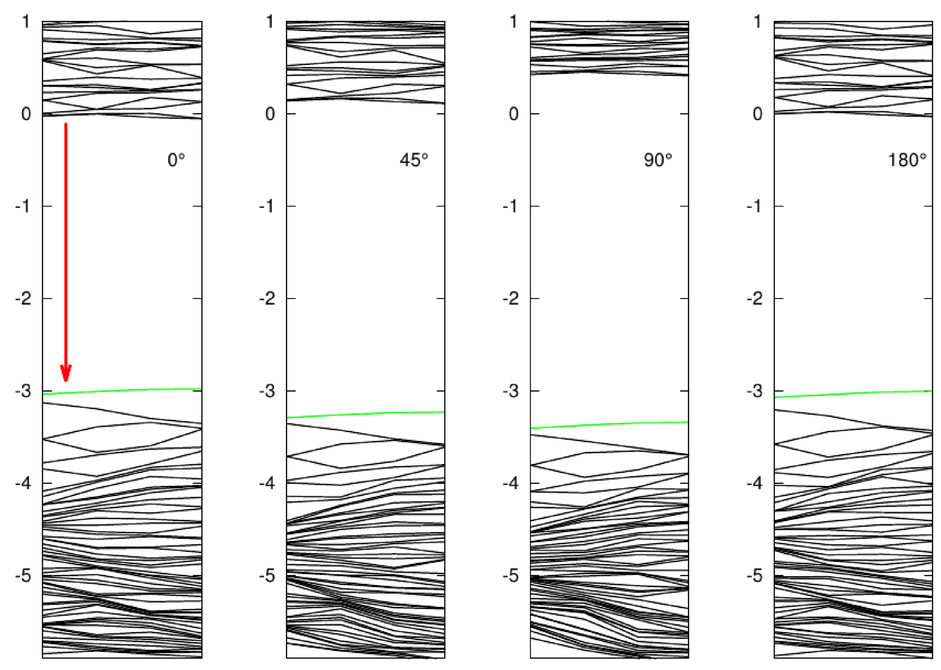
C. Attaccalite, L. Wirtz, A. Marini, and A. Rubio, Physica status solidi (b) **244**, 4288 (2007)

Defects in BN nanostructures

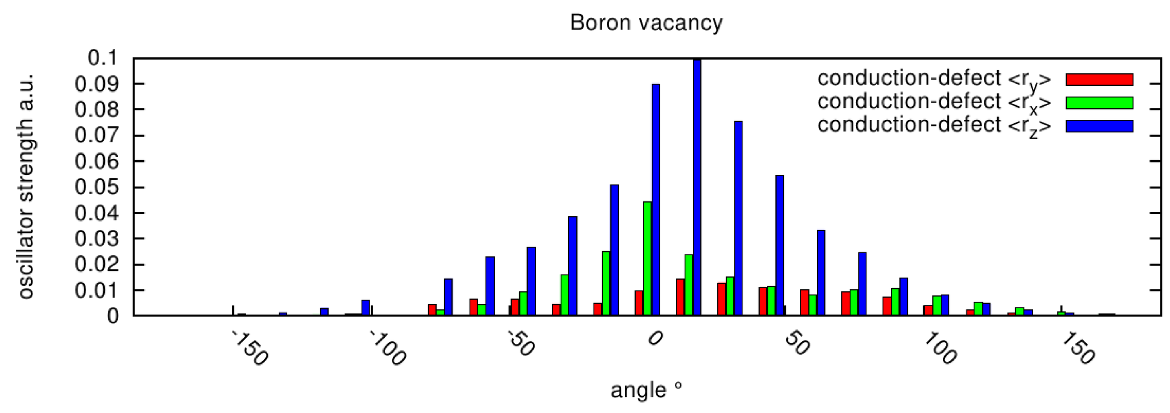




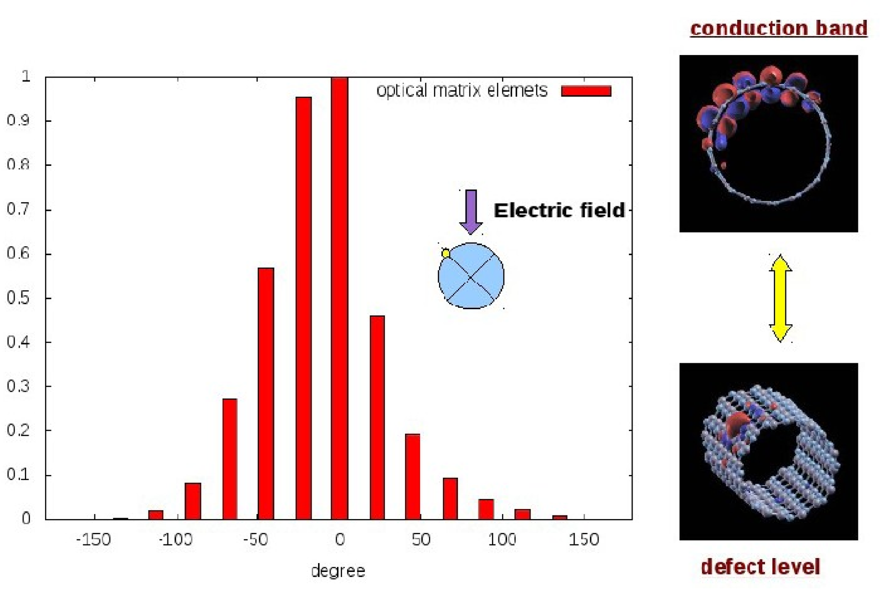
Impurities in BN nanostructures induce light emission below 5 eV, and also affect the luminescence arising from the main bulk exciton. These effects can be explained by the presence of deep levels in the BN band gap.



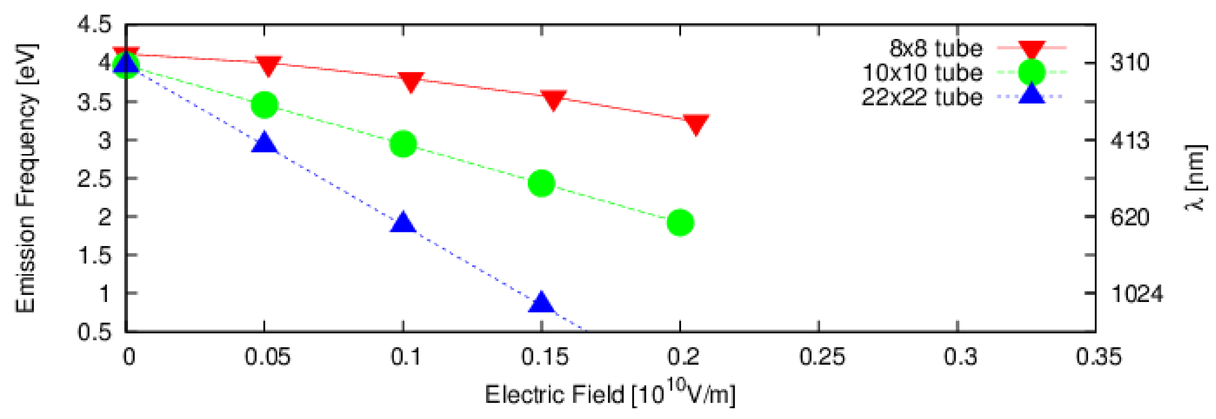
When we turn on a transverse electric field, the band gap of the tube gets shrunk. Nevertheless **the defect levels position in the band gap does not change**. This is due to the fact that the orbitals associated with defect levels are strongly localized on the impurities and therefore are less deformed by the presence of the external field.

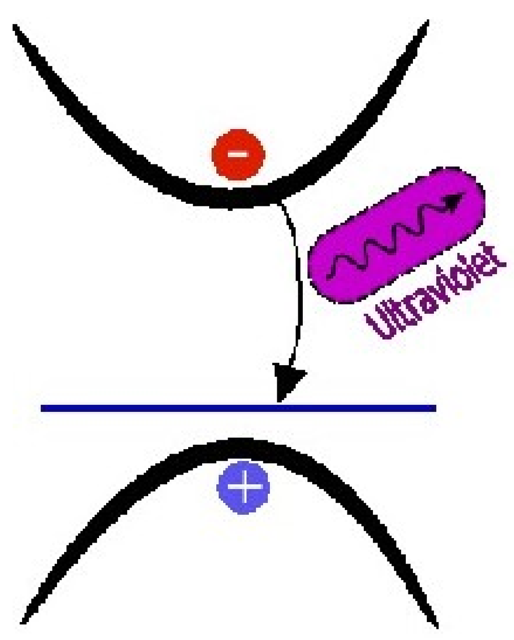


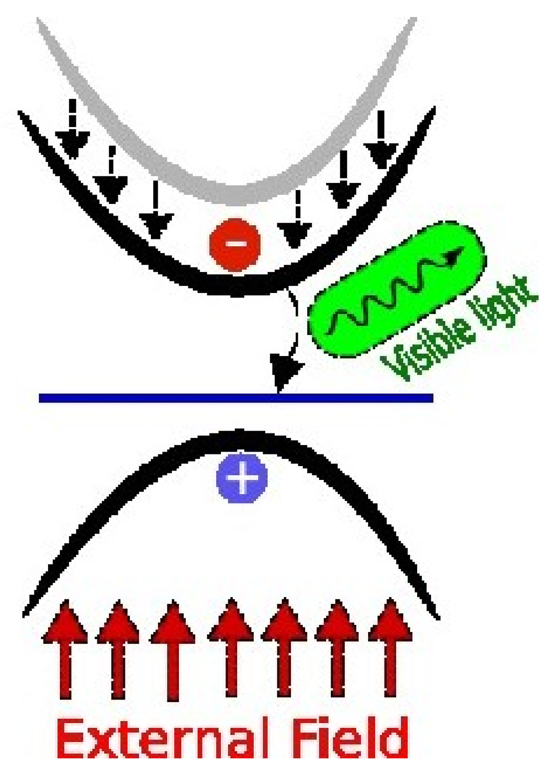
Tuning defects light emission



In order to predict **light emission** we started from the quasi-particle band structure. Then we included the electron-hole attraction between the first conduction band and the defect level. And finally we estimated the Stocks shift by mean of a constrained-DFT calculation.







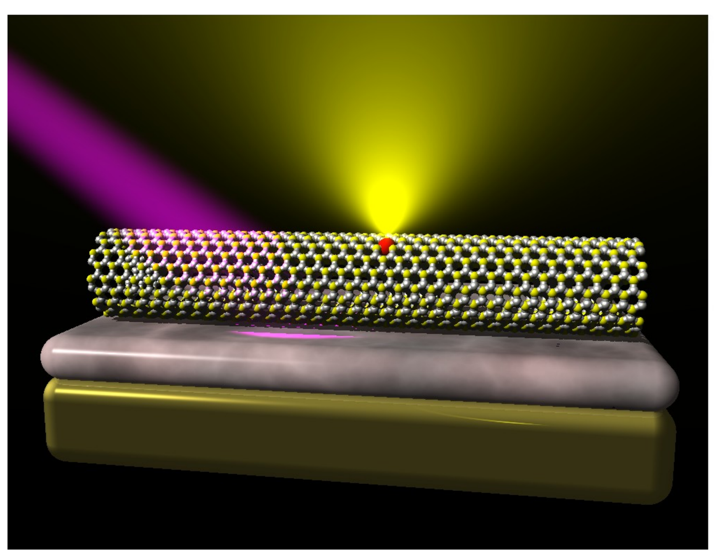
The final device

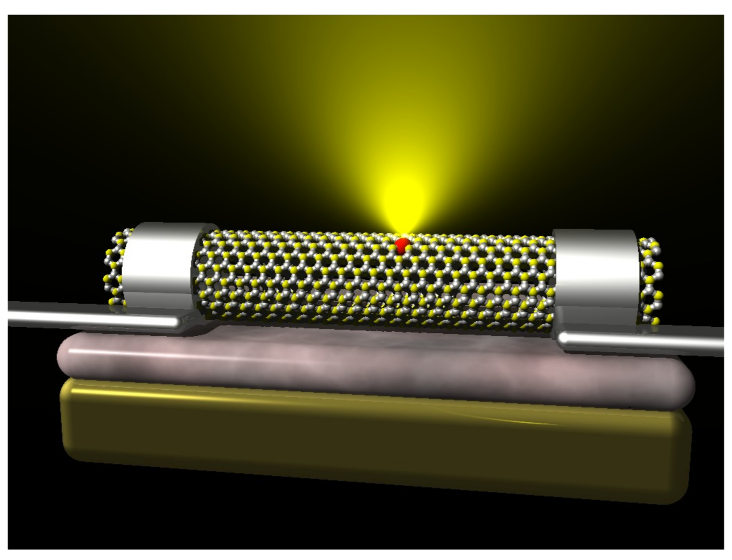
The generic configuration of the device comprises depositing a BN nanotube on an insulating surface acting as a dielectric to enable the application of the gated electric field that controls the light emission.

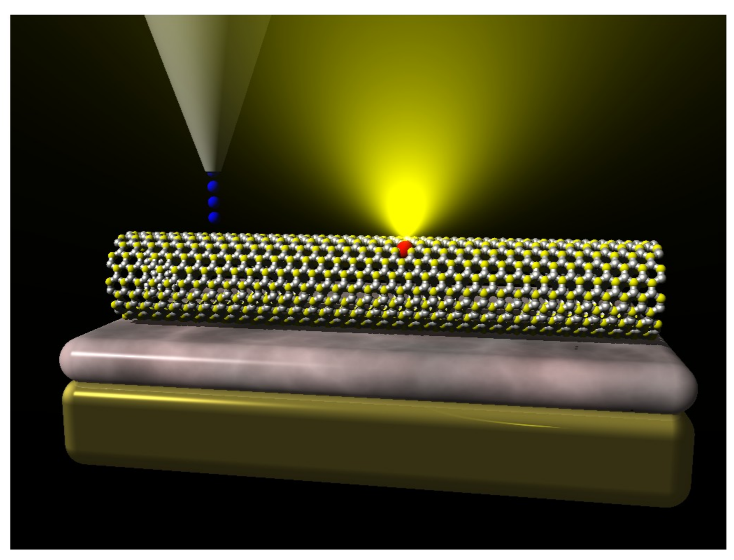
The configurations is very much similar to the one of field effect transistor (FET). The activation of the device could be induced by:

i) introducing an ambipolar current, this current recombines in the defect and emits light dictated by the applied gate voltage

ii) using electrons and or light to excite the nanotube, the excited electrons would decay immediately into the lowest energy state that would further decay by emitting light, again with a frequency dictated by the applied voltage.







LIGHT EMITTING SOURCE AND METHOD FOR EMITTING LIGHT BASED ON BORON NITRIDE NANOTUBES
A RUBIO SECADES, C ATTACCALITE, L WIRTZ
WO Patent 2,012,113,955 (2012)

Calculations performed at CIMENT and IDRIS