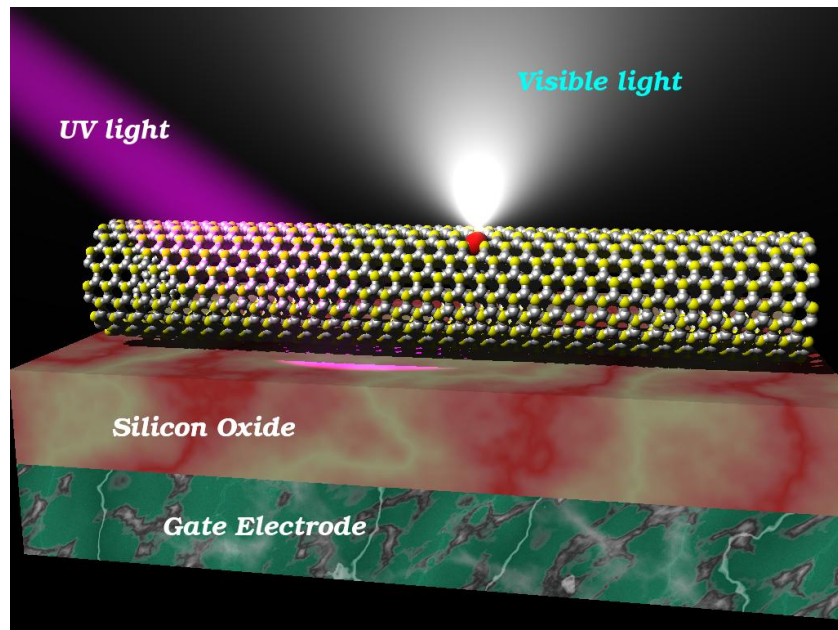


Modeling optoelectronic nanostructured devices made of inorganic nanotubes

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We will review the work done in the group in the last year to characterize and predict the properties of BCN-based nanostructures and address their potential applications. In particular the different spectroscopic techniques that are currently used for BCN-nanostructures. We will present the spectroscopy of hexagonal boron nitride (hBN) (sheet and bulk) and BN nanotubes from a theoretical perspective. The measured Raman spectra can be fully explained by ab-initio simulations of the spectra. For the interpretation of optical absorption and luminescence, a detailed knowledge of the excited state properties is required. We show that BN displays strongly bound excitons whose binding energy increases from three-dimensional hBN, via the 2D single sheet to te quasi -1D BN tubes. However, the excited state properties of the pure structures seem not to explain most of the measured luminescence spectra. Thus, we investigate the influence of different possible defects in hBN such as vacancies, carbon substitutions as well as how BN nanodomains can be incorporated in the grapheme (“nanoscale patchwork”). Furthermore, we present results on the influence of external E-fields on the excitonic spectra of BN tubes. We will discuss potential applications in optoelectronic devices as well as other applications. We will summarize the experimental and theoretical studies in those structures and at the end we will make connections with carbon-based materials, as grapheme/graphite and their interconnections.