Namur Institute of Structured Matter

UNIVERSITÉ DE NAMUR

Seminar

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« Low-frequency vibrations in low-dimensional structures »

When and where:

Thursday December 5th 2019 at 11:00
UNamur, Rue Grafé 2, B-5000 Namur
Chemistry & Physics building
Salle académique (5th floor)

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« Low-frequency vibrations in low-dimensional structures »

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To date, the pool of high-quality two-dimensional (2DMs) and one-dimensional materials (1DMs) continues to grow at an accelerated pace and already covers an extensive range of fascinating and technologically relevant properties. An array of experimental techniques have been developed and used to characterize and understand these properties. In particular, Raman spectroscopy has proven to be a key experimental technique, thanks to its capability to identify minute structural and electronic effects in nondestructive measurements. While high-frequency (HF) intralayer Raman modes have been extensively employed for 1DMs and 2DMs, recent experimental and theoretical progress has demonstrated that low-frequency (LF) Raman modes can be more effective at determining a number of structural properties such as width, length (1DMs) and number of layers, and stacking configurations (2DMs). Compared to HF Raman modes, the relatively small attention originally devoted to LF Raman modes is largely due to their weaker signal and their proximity to the strong Rayleigh line background, which previously made their detection challenging. Recent progress in Raman spectroscopy with technical and hardware upgrades now makes it possible to probe LF modes with a standard single-stage Raman system.

In this talk, I will review my group's contributions to the theoretical and computational understanding of those modes and their behavior as a function of the details of the structures under investigation. I will demonstrate that a quantitative quantum mechanical description of the low-frequency modes can be obtained for a variety of experimentally relevant parameters. I will also show how focusing on LF modes has enabled the prediction of some modes that were then actually observed and rationalized to yield key structural properties of the structures under investigation. Finally, if time permits, I will spend some time describing the phonon properties of twisted graphene bilayers and how shear and breathing modes are unique indicators of twisting angles.