Seminar: Hard Condensed Matter Theory

JOHANNES GUTENBERG UNIVERSITÄT MAINZ

Room: Galilei Raum, 01-128 (Staudinger Weg 9)
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Rafael Gonzalez-Hernandez

Departament of Physics, Universidad del Norte, Barranquilla, Colombia

Computational modeling of 2D materials beyond graphene

The last decade has seen nearly exponential growth in the science and technology of two-dimensional (2D) materials. Beyond graphene, there is a great variety of new monolayer materials, which can adjust their properties from insulators to superconductors. On the other hand, the stacking of different materials also allows an additional "dimensionality" in the design of new semiconductor and superconductor heterostructures. In this talk, I will discuss recent breakthroughs in the theoretical characterization of two-dimensional materials, including the new 2D nitrides. In particular, starting from the wurtzite phase of gallium nitride (GaN); mechanical, electronic and optical properties of a novel 2D phase (type of graphene, known as g-GaN) is debated. The structural and vibrational stability of g-GaN is presented within the density functional theory (DFT) framework [1]. It is also shown a comparative study to reveal how their physical properties are modified by the dimensionality and doping [2].

[1] P. Giannozzi, et al, J. Phys.: Condens. Matter, (2009), 21, 395502

[2] R. González, W. López-Pérez, Á. González-García, M. Moreno-Armenta, R. González-Hernández, Applied Surface Science, (2018) 433,1049

All interested are cordially welcome!