PROGRAMA DE DOCTORADO EN FÍSICA DE LA MATERÍA CONDENSADA, NANOCIENCIA Y BIOFÍSICA

SEMANA DEL DOCTORADO UAM 2025

A QUIEN PUEDA INTERESAR

D. PEDRO JOSÉ DE PABLO GÓMEZ, Coordinador del *Programa de Doctorado Interuniversitario en Física de la Materia Condensada, Nanociencia y Biofísica*, de la Universidad Autónoma de Madrid, la Universidad de Murcia y de la Universidad de Oviedo,

CERTIFICA:

que **D. Gonzalo Nicanor Molina**, ha asistido y participado satisfactoriamente en la Sesión Científica Anual del Programa de Doctorado que ha tenido lugar de forma presencial en la Facultad de Ciencias de la UAM los días 27 y 28 de mayo de 2025, con un total de 16 horas de aprovechamiento.

Y, para que conste a los efectos oportunos, firma el presente documento en Madrid a 3 de Junio de 2025.

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Phonon Dispersion in Hexagonal Boron Nitride: A Continuum Model Approach

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The twisted stacking of layers in van der Waals materials, forming moiré superlattices, has opened up new avenues for exploring the physics of strongly correlated systems and various emergent phenomena. Among these materials, hexagonal boron nitride (hBN), though less well-known than its isostructural counterpart graphene, stands out due to its insulating nature, oxidation resistance, high thermal conductivity, and exceptional mechanical strength. These properties, coupled with the potential to engineer new behaviors through twisted bilayer configurations, position hBN as a versatile material for state-of-the-art applications.

One of the primary challenges in harnessing these applications lies in understanding phonons (propagating atomic vibrational waves), which critically influence a material's thermal, mechanical, optoelectronic, and transport characteristics. Recently, Cappelluti et al. [1] developed a continuum model to describe the lattice dynamics of twisted bilayer graphene, revealing significant band flattening across nearly all high-frequency in-plane lattice vibration modes, including the valley Dirac phonon, valley optical phonon, and central-zone optical phonon bands. This discovery provided new insights into phonon scattering in complex two-dimensional materials.

Building on these findings, our primary objective was to extend this continuum model to other two-dimensional materials, with a particular focus on hBN. In this study, we applied Density Functional Perturbation Theory (DFPT) using the Quantum ESPRESSO package with Perdew–Burke–Ernzerhof (PBE) functionals within the Generalized Gradient Approximation (GGA) and PAW pseudopotentials. This approach allowed us to optimize the structure and obtain phonon dispersion bands for both monolayer hBN and various stacking configurations [2].

As a result, our simulations confirmed the validity of the continuum model for capturing phonon dispersion. Specifically, the continuum model accurately captured the behavior of phonon dispersion at high-symmetry points in the Brillouin zone, including the LO/TO splitting observed in bilayer configurations. This robust representation allowed us to perform a deeper analysis of the phonon dispersion in twisted bilayer hBN, offering valuable insights into its potential for novel and innovative applications.

References

[1] Emmanuele Cappelluti, Jose Angel Silva-Guillén , Habib Rostami, and Francisco Guinea. PHYSICAL REVIEW B 108, 125401, (2023).

[2] Constantinescu, G., Kuc, A., & Heine, T. Stacking in Bulk and Bilayer Hexagonal Boron Nitride. Physical Review Letters, 111(3), (2013).