Vibrational properties of BN polymorphs studied by first-principles calculations

Priyanka Mishra and Nevill Gonzalez Szwacki

Faculty of Physics, University of Warsaw, Pasteura 5, PL-02093 Warsaw, Poland

Boron nitride (BN) is a material with several crystalline polymorphs, large surface area, thermomechanical stability, and excellent thermal conductivity [1]. However, the relative thermodynamic stability of its most common polymorphs has not been experimentally resolved satisfactorily. This lack of understanding hampers the development of potential technological applications [2].

In this work, we use first-principles calculations to study the vibrational properties and relative stability of several BN phases that structurally differ in the arrangement of the constituent BN layers with a honeycomb structure. The phases of our interest are AA-BN and *h*-BN with on-top stacking where the layers are exactly aligned and AB-BN as well as *r*-BN (ABC stacking) in which the layers are shifted with respect to each other. The actual differentiation of structurally similar phases by their vibrational properties is possible (see Fig. 1) but requires very accurate calculations since the phonon frequencies of the layered materials are very close in value. Our theoretical findings therefore should stimulate new experimental efforts that can be combined with high-level calculations.

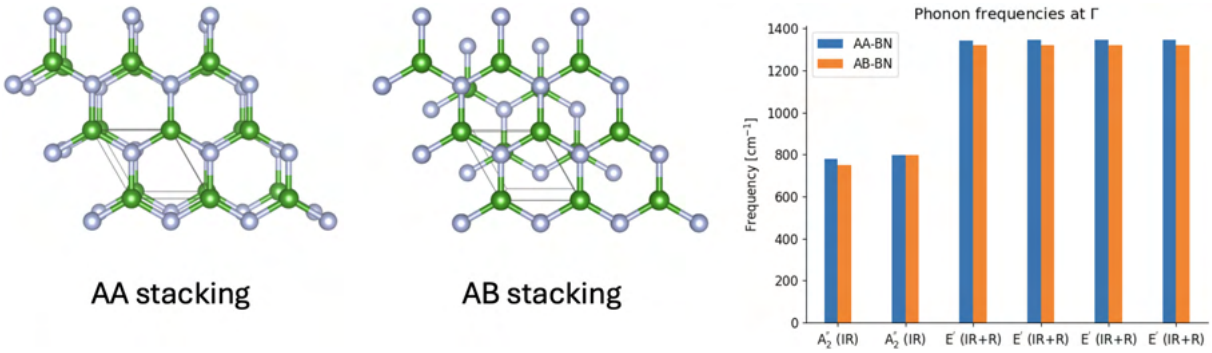

Figure 1: BN polymorphs having $P\bar{6}m2$ space group symmetry. The atomic stacking of the layers is shown (left). The phonon frequencies computed at the Γ point for the relaxed structures are also shown (right).

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[1] P. Tatarczak et al., Nanotechnology **35**, 175703 (2024).

[2] B. Gil et al., Crystals **12**, 782 (2022).