Understanding the lattice dynamics of multilayered h-BN: peculiar infrared optical responses

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Two-dimensional (2D) materials and nano-layered conformations of hexagonal boron nitride (h-BN) can be efficiently used as dielectric counterparts in graphene nanostructures, for lubrication or electronics, or directly replace other materials for high temperature applications [1,2]. Stacking mismatches, nevertheless, could affect the photonic [3], mechanical and thermal properties [4] and, to access information about the stacked configuration of layered ensembles, highly sophisticated and expensive techniques are necessary [5].
A deep understanding of the lattice dynamics of 3D h-BN, instead, could open new perspectives in the clarification of experimental outcomes, e.g. from infrared or Raman spectroscopy [6]. Unfortunately, the task is particularly challenging for the theoretical investigation, because of the great anisotropy of the material [7].
We performed a comprehensive analysis [8] of the lattice dynamics of stacked h-BN comparing different matching variants. We report on different levels of Density Functional Theory (DFT): exchange-correlation functionals, psudopotential approximations (resulting particularly important) and formal van der Waals dispersion corrections, comparing with reviewed experimental results.
From the results of our extensive computational study, it emerges clearly the necessity of a different physical description (we call it complex approach, like a complex number) for the deformations involving mainly the covalent framework and the ones which involve, instead, importantly the interplanar van der Waals interactions. This different approach could be moved to a more fundamental level than how it is, nowadays, implemented in the DFT, resulting extremely effective in 2D systems, stated their geometrical and chemical peculiarity (particularly nitrogen based, and best of all in h-BN).

References

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Figures

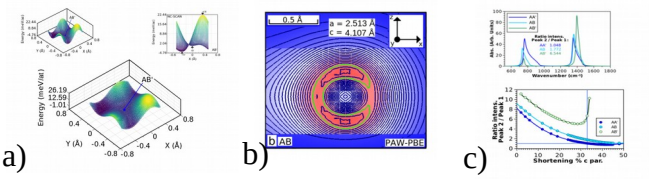

Figure 1: (a) Potential energy surfaces for sliding of contiguous h-BN planes, (b) real space charge density function in the vicinity of a nitrogen atom in an employed h-BN fictitious system of approximation and (c) calculated structure-specific infrared absorption spectra.