# Benchmark calculations of the lattice constant of h-BN

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Hexagonal boron nitride (h-BN) is one of the most studied 2D materials after graphene and yet it has not been determined experimentally or at a satisfying level of theory which of the various possible stacking arrangements are stable and present in experimental samples. A highly accurate determination of the interlayer forces and lattice constants is required to perform reliable lattice dynamics calculations due to the similarity in the electronic structure of the three assumed to be stable stackings (AA', AB, AB' seen in Fig.1). In our work we provide a an ab-initio insight and accurate calculation of properties of bulk hexagonal boron nitride (h-BN) at the density functional theory (DFT) and state of the art Quantum Monte Carlo (QMC) level of electronic structure theory. In our study we focused on the 5 known two layer stacking configurations where we compare the interlayer distances obtained from available DFT dispersion correction methods with those obtained by experiment and QMC. We also present equilibrium lattice constants and interlayer binding energies obtained by standard relaxation algorithms compared with a detailed scan of the potential energy surface (PES). By scanning the PES we are able to asses the level of accuracy to which one can reliably calculate the lattice constants.

## References

[1] F. Hummel, T. Gruber, and A. Grüneis, Eur. Phys. J. B 89, 235 (2016)
[2] I.V. Lebedeva, A.V. Lebedev, A.M. Popov, and A.A. Knizhnik, Comp. Mat. Sci.128, 45 (2017).
[3] 3 C.-R. Hsing, C. Cheng, J.-P. Chou, C.-M. Chang, and C.-M. Wei, New J. Phys. 16, 113015 (2014).
[4] Harrison, H., et al., Nanoscale Advances 1.5 (2019): 1693-1701.
[5] Ohba, N., et al., Phys. Rev. B 63.11 (2001): 115207.

## Figures

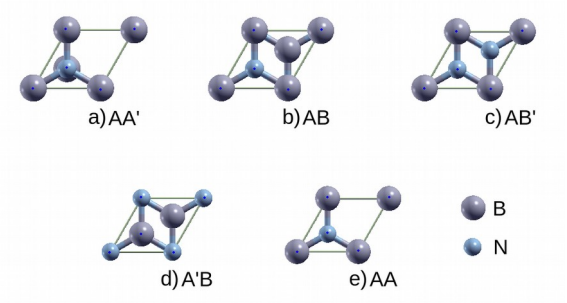


**Figure 1:** Five different stacking orders in hexagonal boronnitride