2D Hexagonal Boron Nitride

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Introduction

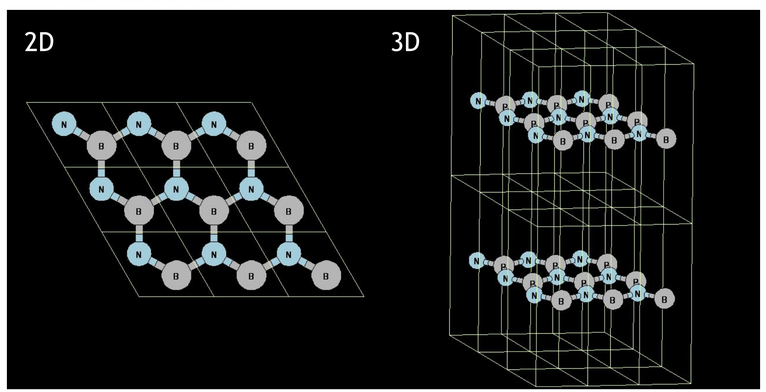
Hexagonal Boron Nitride (h-BN) has encountered much attention in recent times due to its incredible electrical, thermal, and mechanical properties. We investigate 2D h-BN through DFT to track a new trend of increasing interlayer spacing a function of the number of layers seen below. Our interest in h-BN stems from its use as a deep UV photodetector (200-280 nm).

	Total Number of Layers	Interlayer Spacing (nm)
Measured	2	0.515
	3	0.436
	4	0.412
	5	0.400
	10	0.347
	27	0.333
Theoretical/experimental	Bulk	0.331-0.333

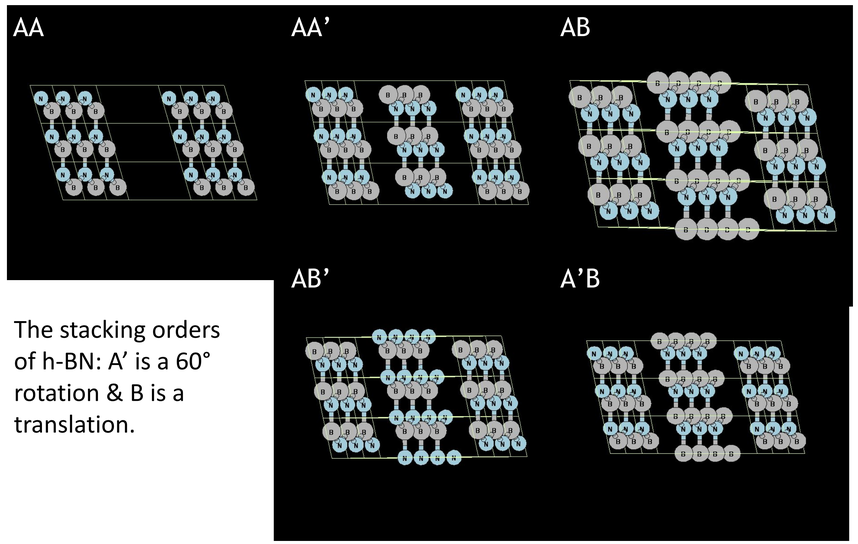
The total number of layers from bulk to bilayer forms have different interlayer spacing, from 0.515 to 0.33 nm respectively.

Methods & System Description

- PBEsol + DFT-D3
- Energy Cutoff 80 Ry
- Charge Density Cutoff 800 Ry
- K-Points: 12 x 12 x 4



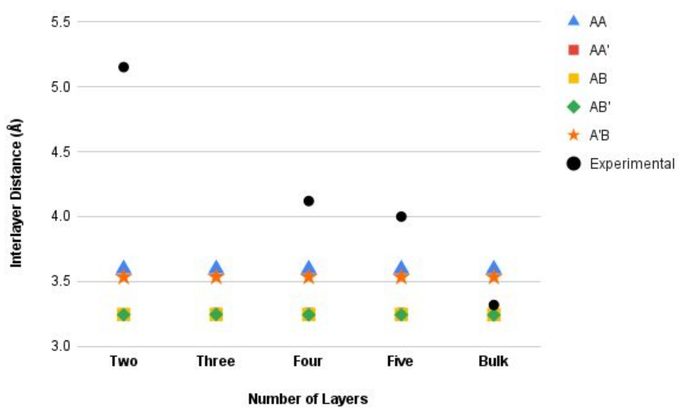
Taken from XCrySDen of the lattice structure of h-BN both in 2D (left) and 3D (right) forms. Blue atoms are Nitrogen, pink atoms are Boron.

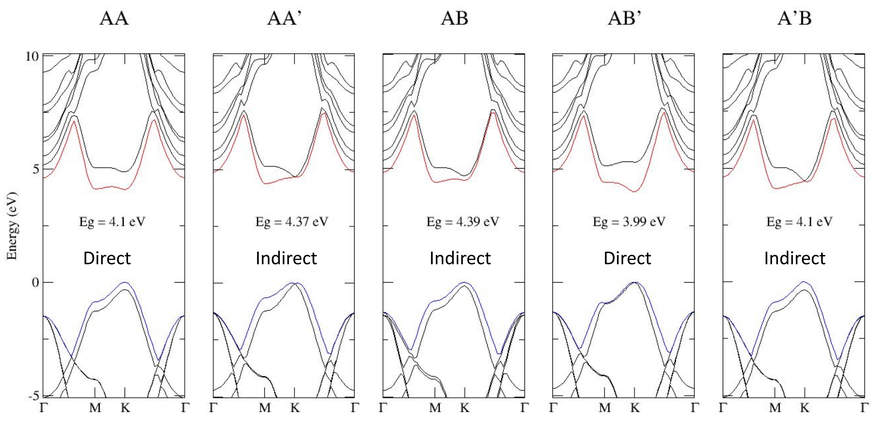


The stacking orders of h-BN: A' is a 60° rotation & B is a translation.

Results

The measured and calculated interlayer distances as a function of the total number of layers. our theoretical results are unable to reproduce experimental findings. DFT finds non-varying interlayer distances across all five stacking orders when decreasing the number of from bulk to two layers on the order of a hundredth or thousandth of an Ångstroms





The electronic band structure of bilayer h-BN: AA, AA', AB, AB', and A'B, from left to right. Conduction band in red and valence band in blue. AA' and AB are of similar band gap energy and higher in magnitude than AA, AB', and A'B who are all also similar in magnitude.

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