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 as 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).

<table>
<thead>
<tr>
<th>Total Number of Layers</th>
<th>Interlayer Spacing (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Measured</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>0.515</td>
</tr>
<tr>
<td>3</td>
<td>0.436</td>
</tr>
<tr>
<td>4</td>
<td>0.412</td>
</tr>
<tr>
<td>5</td>
<td>0.400</td>
</tr>
<tr>
<td>10</td>
<td>0.347</td>
</tr>
<tr>
<td>27</td>
<td>0.333</td>
</tr>
<tr>
<td>Theoretical/experimental</td>
<td>0.331-0.333</td>
</tr>
</tbody>
</table>

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

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.

Acknowledgements

Special thanks to Dr. Pamuk and Dr. Zhou for their assistance in this project. This work is supported by the National Science Foundation, Platform for the Accelerated Realization, Analysis and Discovery of Interface Materials (PARADIM). Questions can be directed to nimitmishra@ucla.edu

References