New Paltz STATE UNIVERSITY OF NEW YORK — Particle–Hole Asymmetry in h-BN explained by NNN Tight-Binding

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Hexagonal boron nitride (h-BN) is atomically flat, chemically inert, and has a wide band gap (about 6 eV), which suppresses interface traps and yields low, reproducible leakage even at nanometer thickness. We connect these device-level advantages to a compact tight-binding description of the π bands using nearest-neighbor hopping plus a single next-nearest-neighbor term. This minimal model captures **particle–hole asymmetry** and realistic band curvature away from K. Using the evanescent solutions of the two-band dispersion in a tunneling picture, we explain why monolayer h-BN provides stable, low-leakage insulation in 2D heterostructures.

Quantum Mechanical approach to hBN - Tigh Binding

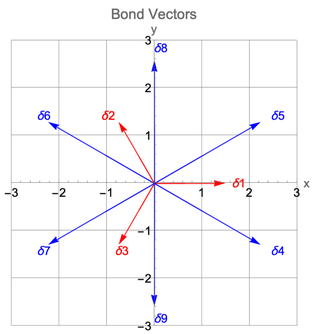

Figure 1. The vectors to Nearest (red) and Next Nearest Neighbors (Blue) in an hexagonal lattice.

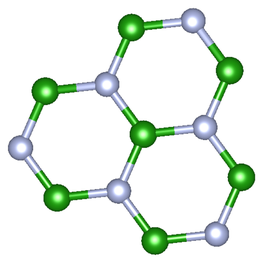

Figure 2. Hexagonal Boron Nitride

The primitive lattice vectors in real space:

$$\mathbf{a}_1 = a\left(\frac{3}{2}, -\frac{\sqrt{3}}{2}\right), \tag{1}$$

$$\mathbf{a}_2 = a\left(\frac{3}{2}, \frac{\sqrt{3}}{2}\right). \tag{2}$$

Structure Factors

- **NN structure factor:** or crystal momentum $\mathbf{k} = (k_x, k_y)$, the nearest–neighbour structure factor is

$$\gamma(\mathbf{k}) = \exp\big(i\,\mathbf{k}\cdot\delta_1\big) + \exp\big(i\,\mathbf{k}\cdot\delta_2\big) + \exp\big(i\,\mathbf{k}\cdot\delta_3\big). \tag{3}$$

- **NNN structure factor**:

$$g(\mathbf{k}) = 2\Big[\cos\big(\mathbf{k}\cdot\mathbf{a}_1\big) + \cos\big(\mathbf{k}\cdot\mathbf{a}_2\big) + \cos\big(\mathbf{k}\cdot(\mathbf{a}_2 - \mathbf{a}_1)\big)\Big]. \tag{4}$$

A simple 2×2 Eigenvalue problem

In the basis (A, B), the momentum–space Hamiltonian is the 2×2 matrix

$$H(\mathbf{k}) = \begin{pmatrix} \frac{\Delta}{2} + t_{2A}\, g(\mathbf{k}) & t\,\gamma(\mathbf{k}) \\ t\,\gamma^*(\mathbf{k}) & -\frac{\Delta}{2} + t_{2B}\, g(\mathbf{k}) \end{pmatrix}. \tag{5}$$

• Off-Diagonal Elements: Describe hopping between nearest neighbors on different sub-lattices. • Diagonal Elements: Contain the on-site energy difference $\pm\Delta/2$ and the NNN hopping inside each sub-lattice.

The two energy bands are obtained by diagonalizing the Hamiltonian matrix:

$$E_\pm(\mathbf{k}) = \frac{1}{2}\Big[\Big(\tfrac{\Delta}{2} + t_{2A}g(\mathbf{k})\Big) + \Big(-\tfrac{\Delta}{2} + t_{2B}g(\mathbf{k})\Big)\Big] \pm \frac{1}{2}\sqrt{\Big[\Big(\tfrac{\Delta}{2} + t_{2A}g(\mathbf{k})\Big) - \Big(-\tfrac{\Delta}{2} + t_{2B}g(\mathbf{k})\Big)\Big]^2 + 4t^2\big|\gamma(\mathbf{k})\big|^2}. \tag{6}$$

How the band edges change with NN and NNN approach

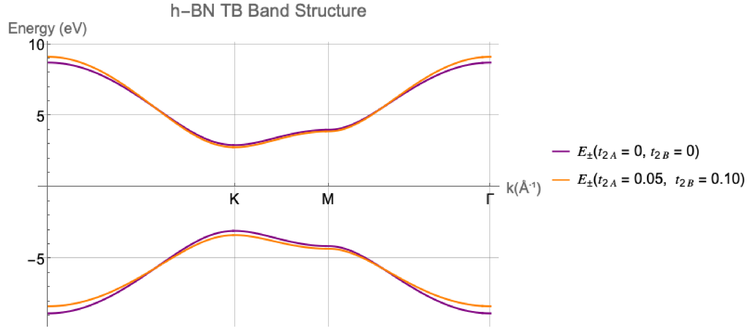

Figure 3. Band Structure comparison between NN and NNN models

Calculations were performed in Wolfram Mathematica, and the code is available at `https://kimreyesg.github.io/research.html`.

The asymmetry field $A(\mathbf{k}) = E_+ + E_-$

$$A(\mathbf{k}) = (t_{2A} + t_{2B})\,\big[g(\mathbf{k}) + 3\big]. \tag{7}$$

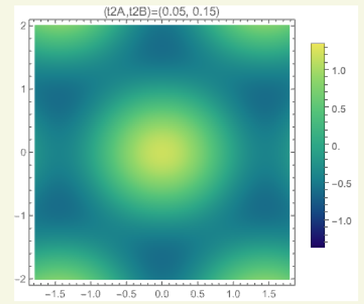

Figure 4. Heat map asymmetry in h-BN when $t_{2A} \neq t_{2B} \neq 0$

Final Results

- The band asymmetry in hexagonal boron nitride (h-BN) comes from inequivalent sublattices: when the on-site terms are different, the “plus” and “minus” bands are not equally spaced about the midline, so the band structure becomes asymmetric around the gap.
- Next-nearest-neighbor terms ($t_{2A} \neq t_{2B}$) can add additional asymmetry, while the nearest-neighbor hopping t mainly controls how fast the bands diverge away from the K point (it changes the slope or curvature there), not the asymmetry at the midline itself.

References

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[2] Akanksha Urade. How is hexagonal boron nitride (hbn) used? AZoNano, October 2022. URL `https://www.azonano.com/article.aspx?ArticleID=6231`. Reviewed by Megan Craig, M.Sc.; accessed 2026-01-10.

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