- # Bilayer Graphene Gap Enhancement Via Substrate Interaction

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Electron Band Gap

Create electron confinement

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- Impurities

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- Quantum dots

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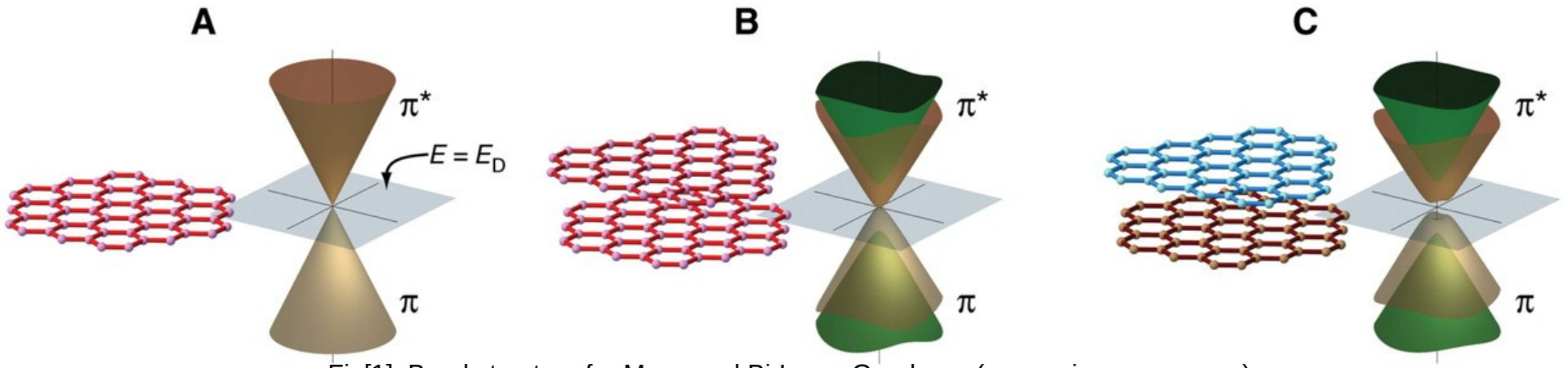
- Nanoribbons

Electron Band Gap

Create electron confinement

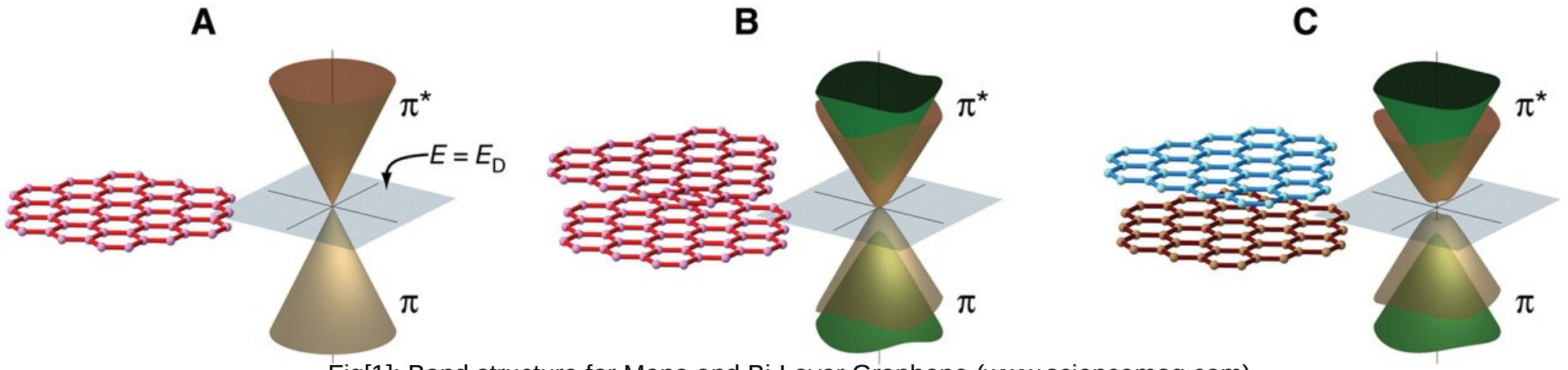
- Impurities
- Quantum dots
- Nanoribbons
- Electron-phonon interaction?

Bilayer Graphene



Fig[1]: Band structure for Mono and Bi-Layer Graphene (www.sciencemag.com)

Bilayer Graphene



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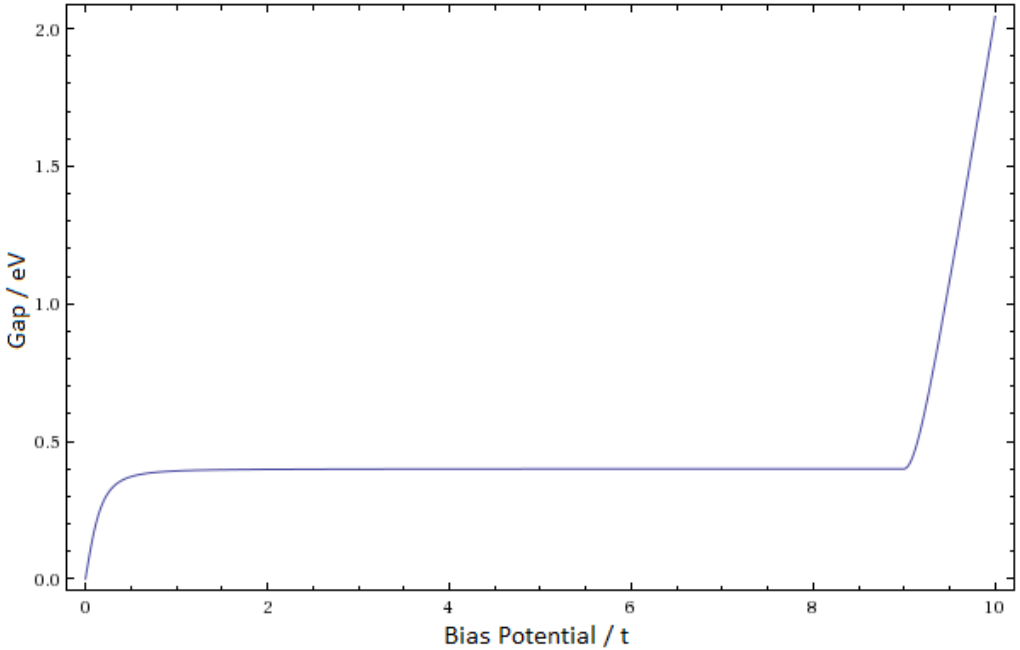
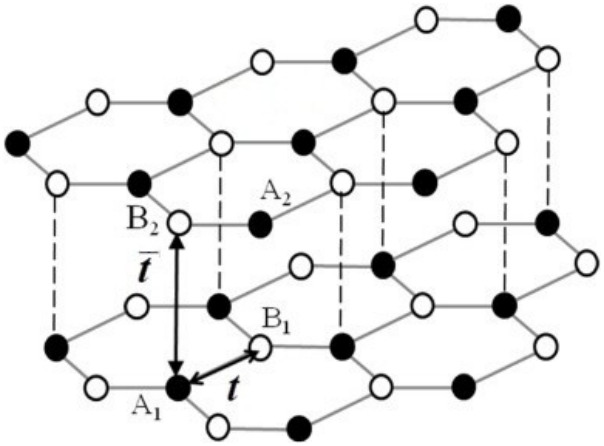


Fig[2]: Electron gap as a function of bias potential, created in Mathematica

Hamiltonian



Fig[3]: Bilayer graphene lattice structure (Rev Mod Phys 81 109)

$$H = -t \sum_{\langle n,n' \rangle \sigma} (a^{\dagger}_{n\sigma} b_{n'\sigma} + b^{\dagger}_{n'\sigma} a_{n\sigma}) - \bar{t} \sum_{\sigma} (a^{\dagger}_{1\sigma} b_{2\sigma} + b^{\dagger}_{2\sigma} a_{1\sigma})$$

$$- \sum_{mn\sigma} f_n(m) n_{n\sigma} \xi_m + \sum_{m} \hbar\omega_0 (N_m + \frac{1}{2})$$

$$+ \sum_{n\sigma} \Delta_n n_{n\sigma}$$

Green's Functions

$$\mathbf{G}_0^{-1}(k, i\omega_n) = [I i\omega_n - H]$$

$$\Sigma(i\omega_n) \approx \begin{pmatrix} i\omega_n(1-Z_n)+\Delta_n & 0 & 0 & 0 \\ 0 & i\omega_n(1-\tilde{Z}_n)+\tilde{\Delta}_n & 0 & 0 \\ 0 & 0 & i\omega_n(1-\tilde{Z}_n)-\tilde{\Delta}_n & 0 \\ 0 & 0 & 0 & i\omega_n(1-Z_n)-\Delta_n \end{pmatrix}$$

$$\mathbf{G}^{-1}(k, i\omega_n) = \mathbf{G}_0^{-1}(k, i\omega_n) - \Sigma(i\omega_n)$$

$$\Sigma_{ii}(\boldsymbol{k}, i\omega_n) = -Tt\lambda \sum_{i\omega_s} \int \frac{d^2\boldsymbol{q}}{V_{BZ}} \mathbf{G}_{ii}(\boldsymbol{k}-\boldsymbol{q}, i\omega_{n-s}) d_0(\boldsymbol{q}, \omega_s)$$

The Solution

$$\Delta_n = 2\delta - t\lambda k_B T \sum_s \int d\epsilon D(\epsilon) \frac{\epsilon^2 \bar{\Delta}'_f - \Delta'_f(\bar{\Delta}'^2_f + \omega_f^2 \bar{Z}_f^2)}{\epsilon^4 + \epsilon^2(-2\Delta'_f\bar{\Delta}'_f + 2\omega_f^2 Z_f \bar{Z}_f) + (\bar{t}^2 + \Delta'^2_f + \omega_f^2 Z_f^2)(\Delta'^2_f + \omega_f^2 Z_f^2)} d_0(i\omega_s)$$

$$\bar{\Delta}_n = 2\bar{\delta} - t\lambda k_B T \sum_s \int d\epsilon D(\epsilon) \frac{\epsilon^2 \Delta'_f - \bar{\Delta}'_f(\bar{t} + \Delta'^2_f + \omega_f^2 Z_f^2)}{\epsilon^4 + \epsilon^2(-2\Delta'_f\bar{\Delta}'_f + 2\omega_f^2 Z_f \bar{Z}_f) + (\bar{t}^2 + \Delta'^2_f + \omega_f^2 Z_f^2)(\Delta'^2_f + \omega_f^2 Z_f^2)} d_0(i\omega_s)$$

$$\delta = t\lambda k_B T \sum_n \int d\epsilon D(\epsilon) \frac{\epsilon^2 \bar{\Delta}'_n - \Delta'_n(\bar{\Delta}'^2_n + \omega_n^2 \bar{Z}_n^2)}{\epsilon^4 + \epsilon^2(-2\Delta'_n\bar{\Delta}'_n + 2\omega_n^2 Z_f \bar{Z}_n) + (\bar{t}^2 + \Delta'^2_n + \omega_n^2 Z_n^2)(\Delta'^2_n + \omega_f^2 Z_n^2)}$$

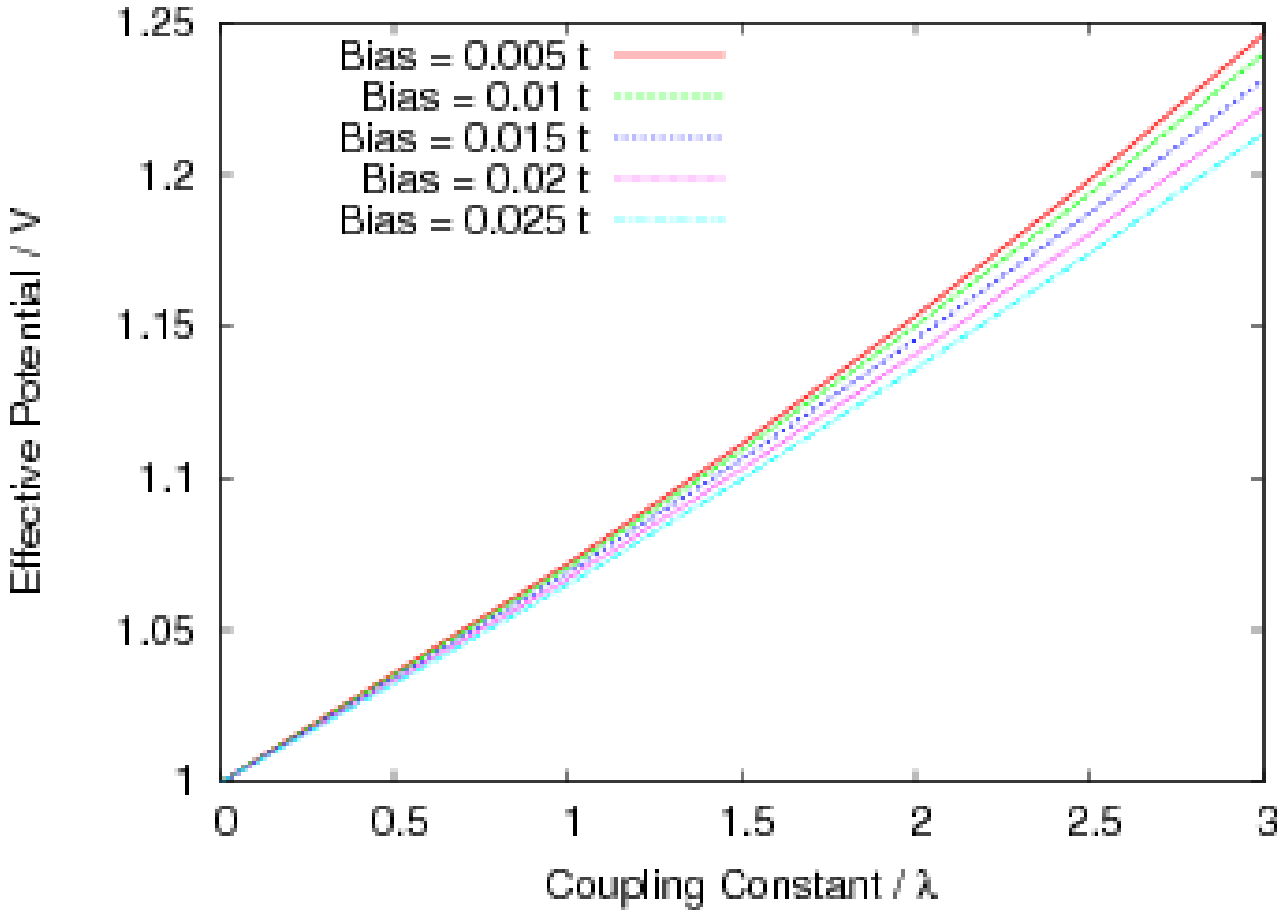
$$\bar{\delta} = t\lambda k_B T \sum_n \int d\epsilon D(\epsilon) \frac{\epsilon^2 \Delta'_n - \bar{\Delta}'_n(\bar{t} + \Delta'^2_n + \omega_n^2 Z_n^2)}{\epsilon^4 + \epsilon^2(-2\Delta'_n\bar{\Delta}'_n + 2\omega_n^2 Z_f \bar{Z}_n) + (\bar{t}^2 + \Delta'^2_n + \omega_n^2 Z_n^2)(\Delta'^2_n + \omega_f^2 Z_n^2)}$$

$$f = n - s$$

$$\Delta' = \Delta + V$$

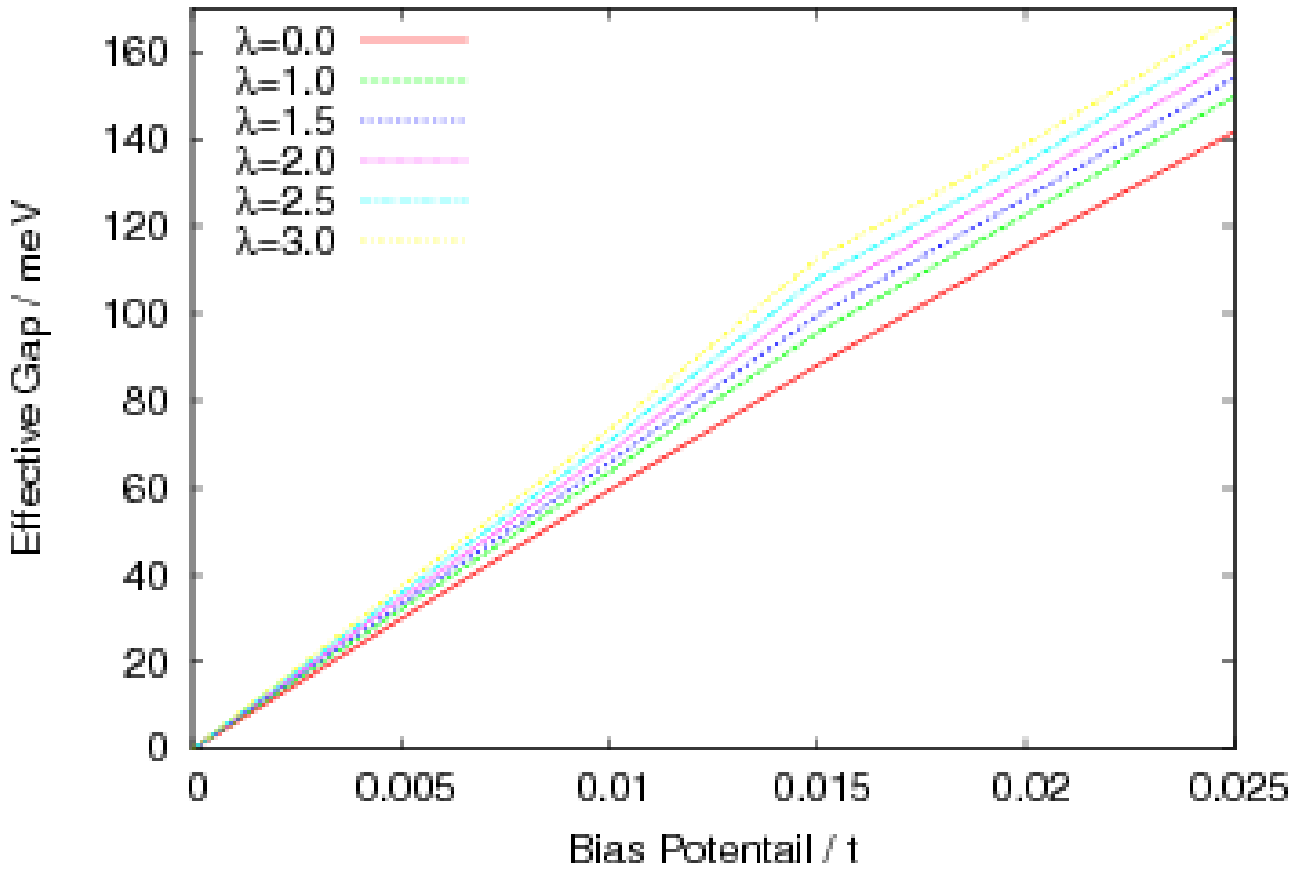
Potential Enhancement

- T = 0.01
  324K
- Ω = 0.01
  ≈ 28meV
- λ = 1.0-3.0



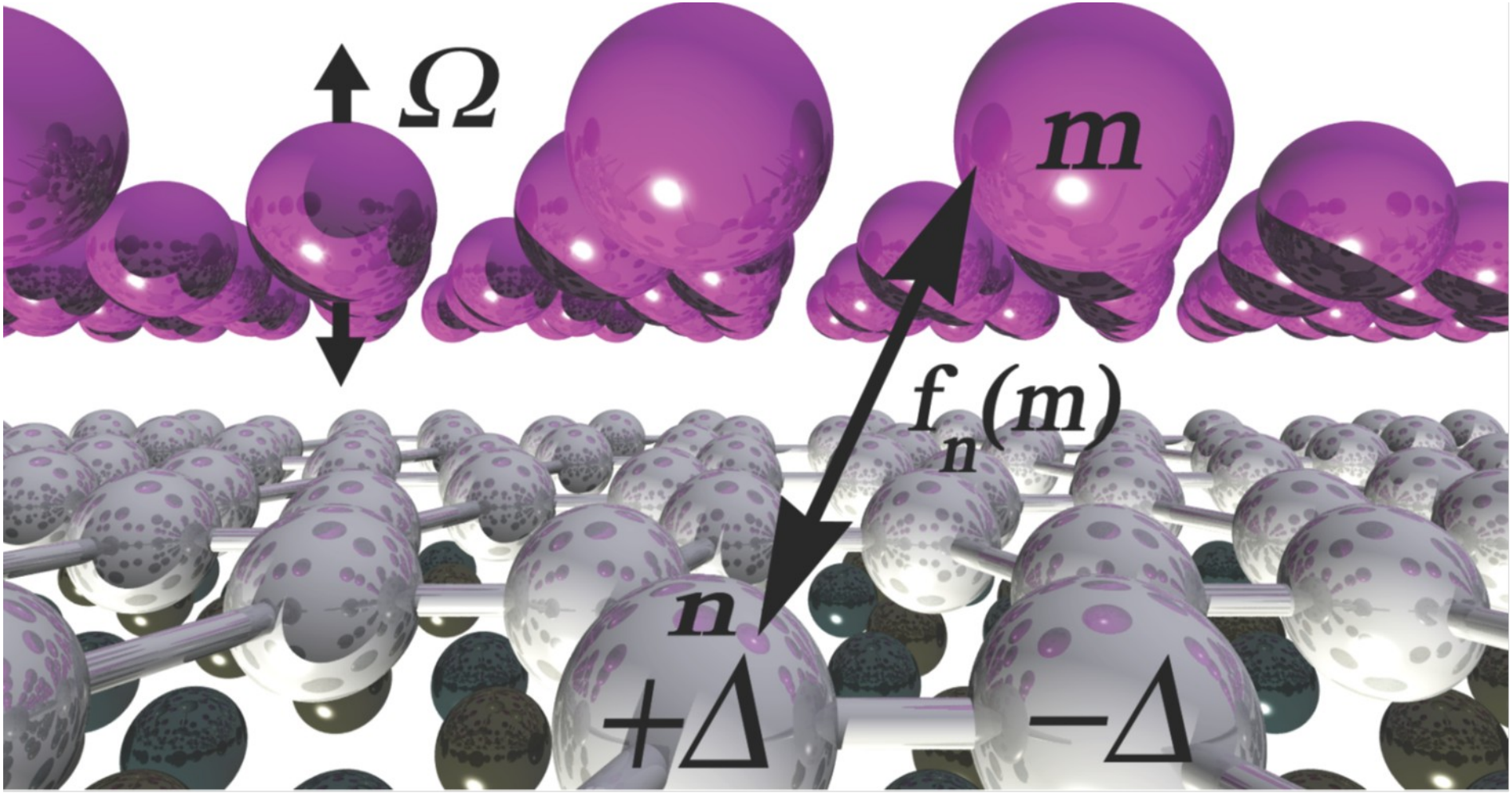
Fig[4]: Bilayer graphene electron-phonon potential enhancement

Gap Enhancement



Fig[5]: Bilayer graphene electron-phonon potential enhancement mapped onto a tight binding model to gain effective gap

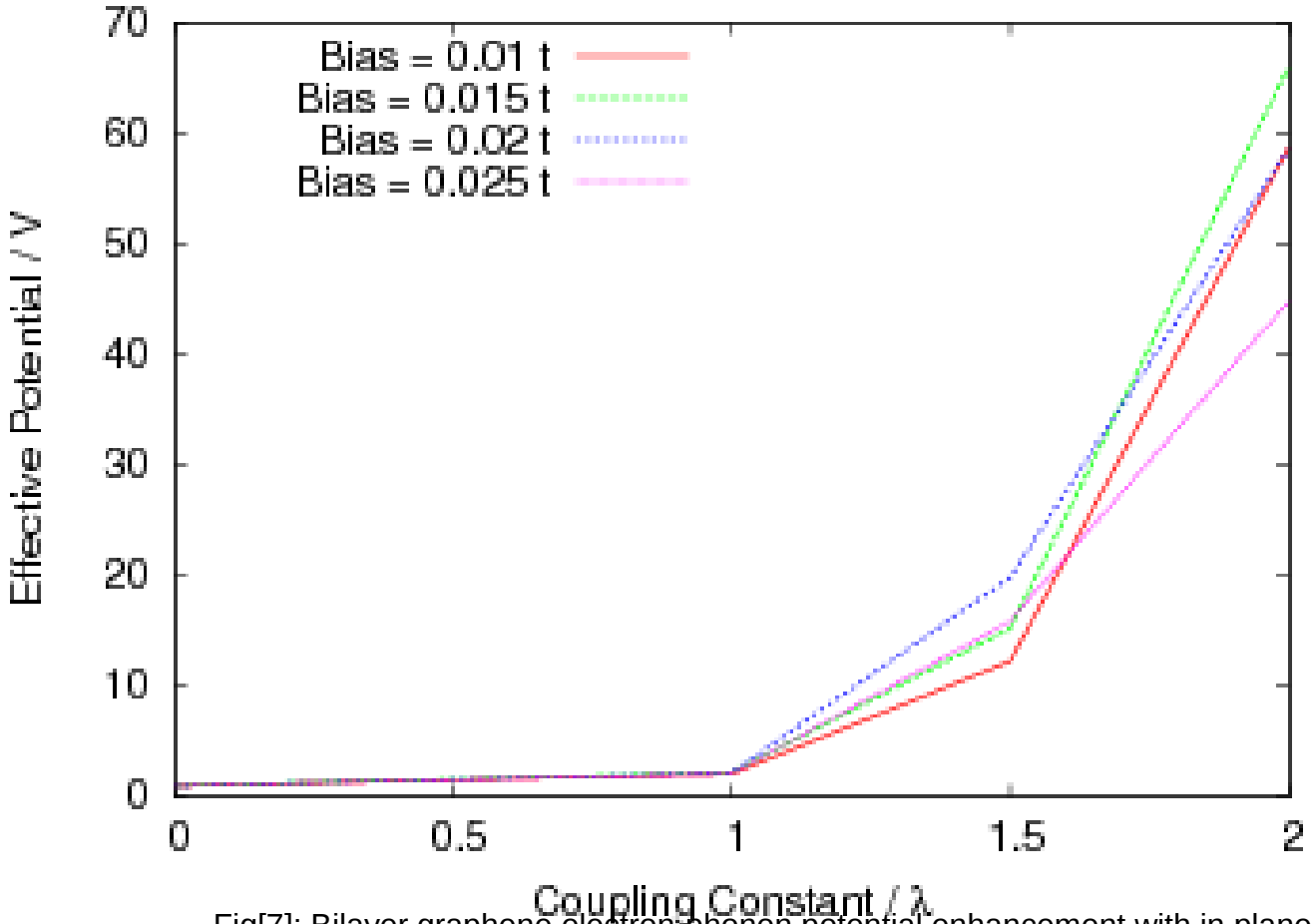
Different Site Potentials



Fig[6]: Creating a in-plane bias potential in addition to a inter-plane bias (Phys Rev B 84 155438)

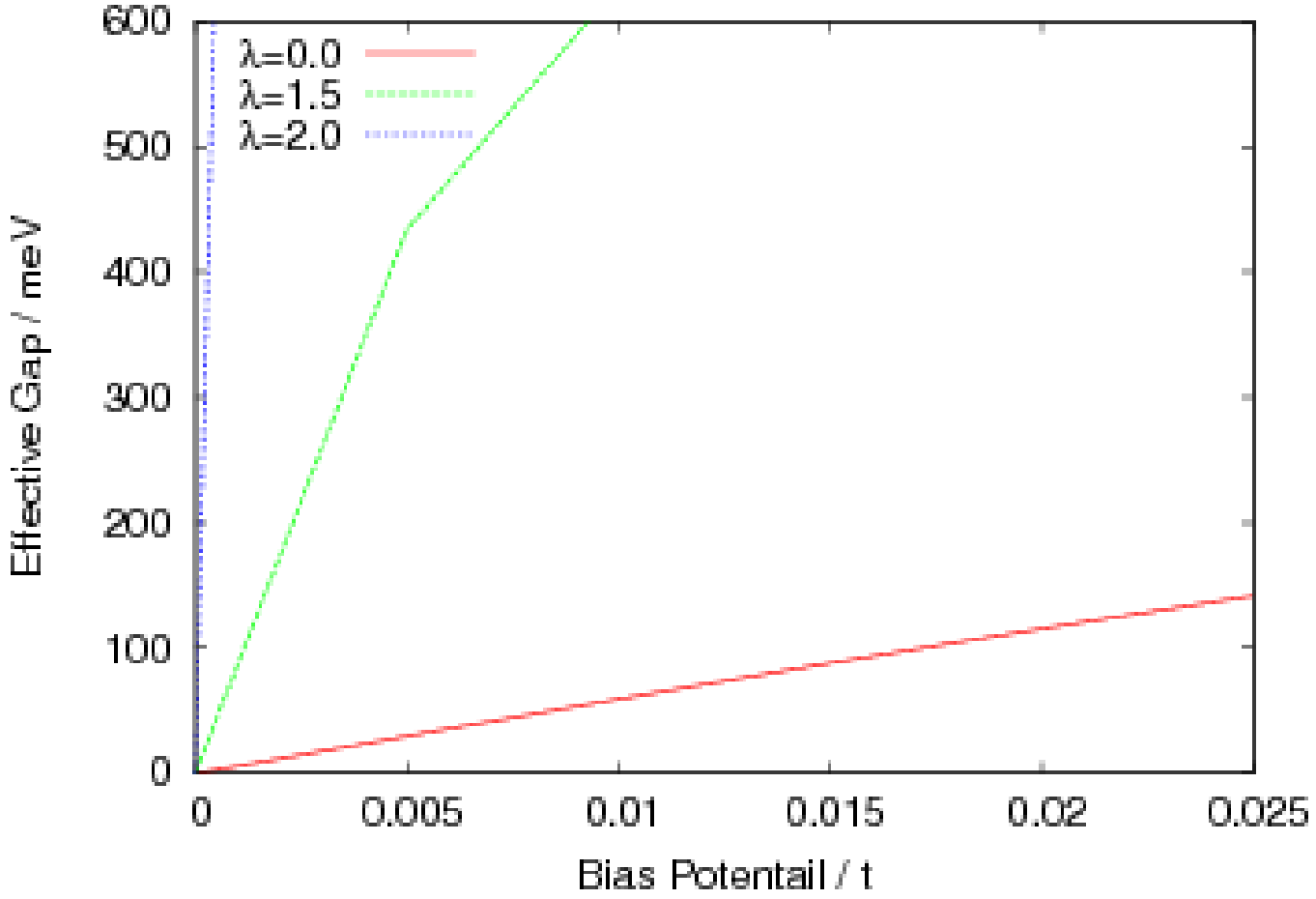
Potential Enhancement

- T = 0.01
  324K
- Ω = 0.01
  ≈ 28meV
- λ = 1.0
- V` = 20%



Fig[7]: Bilayer graphene electron-phonon potential enhancement with in plane bias

Gap Enhancement



Fig[8]: Bilayer graphene electron-phonon potential enhancement mapped onto a tight binding model to gain effective gap with in-plane bias

Summary

- Electron-phonon interactions in biased bilayer graphene has little effect on the band gap
- Slight differences in the site potentials are drastically increased with high electron-phonon coupling
- Large opposing effective potentials create large band gaps
- Bilayer graphitic materials may be better than bilayer graphene