Study of Linear and Nonlinear Optical Properties of Graphene Based on the Dirac Equation

Bahram Parsa

Supervisor:

Dr. Ehsan koushki

Dr. Javad Baedi

Outline

1 • Introduction of klein-Gordon and Dirac equation

2 • Introduction of graphene

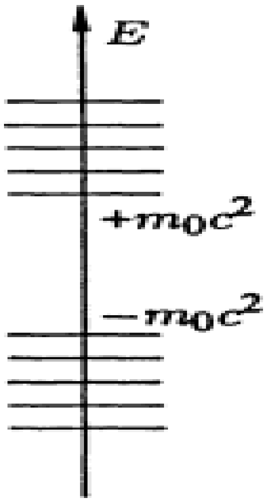
3 • Method

4 • Result

Relativistic wave equation or Klein-Gordon equation

- ✓ $i\hbar \frac{\partial \psi}{\partial t} = \left[-\frac{\hbar^2}{2m_0} \nabla^2 + V(x) \right] \psi(x,t)$
- ✓ $\hat{E} = \frac{\hat{p}^2}{2m_0} + V(x)$
- ✓ $p^\mu p_\mu = \frac{E^2}{c^2} - p \cdot p = m_0^2 c^2$
- ✓ $\hat{p}^\mu \hat{p}_\mu \psi = m_0^2 c^2 \psi$
- ✓ $\varrho = \frac{i\hbar}{2m_0 c^2} \left(\psi^* \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^*}{\partial t} \right)$

  Probability density



Dirac equation

- Dirac Equation an Overview:

✓ $\hat{p}^{\mu}\hat{p}_{\mu} = m_0^2 c^2$

✓ $\hat{p}^{\mu}\hat{p}_{\mu} - m^2c^2 = (\beta^k p_k + mc)(\gamma^{\lambda} p_{\lambda} - mc)$

✓ $(p^0)^2 - (p^1)^2 - (p^2)^2 - (p^3)^2 = (\gamma^0)^2(p^0)^2 + (\gamma^1)^2(p^1)^2 + (\gamma^2)^2(p^2)^2$

$+ (\gamma^3)^2(p^3)^2 + (\gamma^0\gamma^1 + \gamma^1\gamma^0)p_0p_1 + (\gamma^0\gamma^2 + \gamma^2\gamma^0)p_0p_2 + (\gamma^0\gamma^3$

$+ \gamma^3\gamma^0)p_0p_2 + (\gamma^1\gamma^2 + \gamma^2\gamma^1)p_1p_2 + (\gamma^1\gamma^3 + \gamma^3\gamma^1)p_1p_3 + (\gamma^2\gamma^3$

$+ \gamma^3\gamma^2)p_2p_3$

Dirac equation

- ✓ Puli matrix

$$\gamma^0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad \gamma^i = \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix}$$

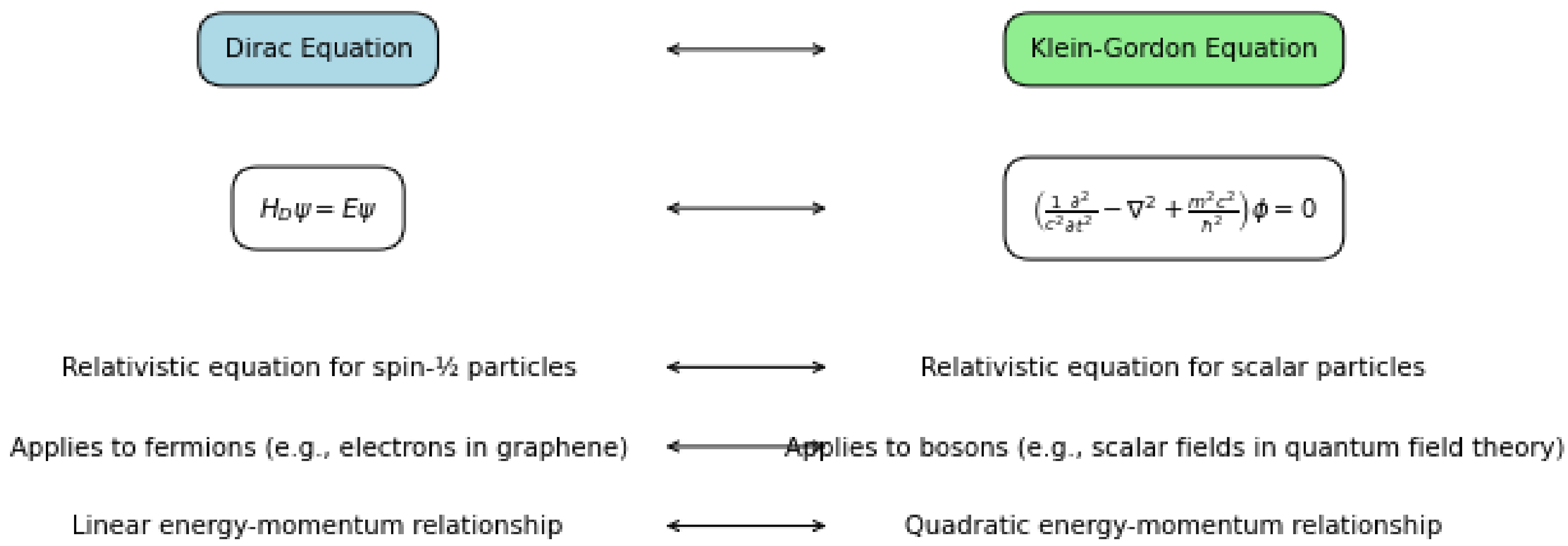
- ✓ the energy and momentum factor

$$\left(\hat{p}^\mu \hat{p}_\mu - m^2 c^2\right) = \left(\beta^k p_k + mc\right)\left(\gamma^\lambda p_\lambda - mc\right) = 0$$

- ✓ The dirac final equation

$$i\hbar\gamma^\mu \partial_\mu \psi - mc\psi = 0$$

Visual Comparision:
Dirac vs. Klein-Gordon Equaion



Graphene

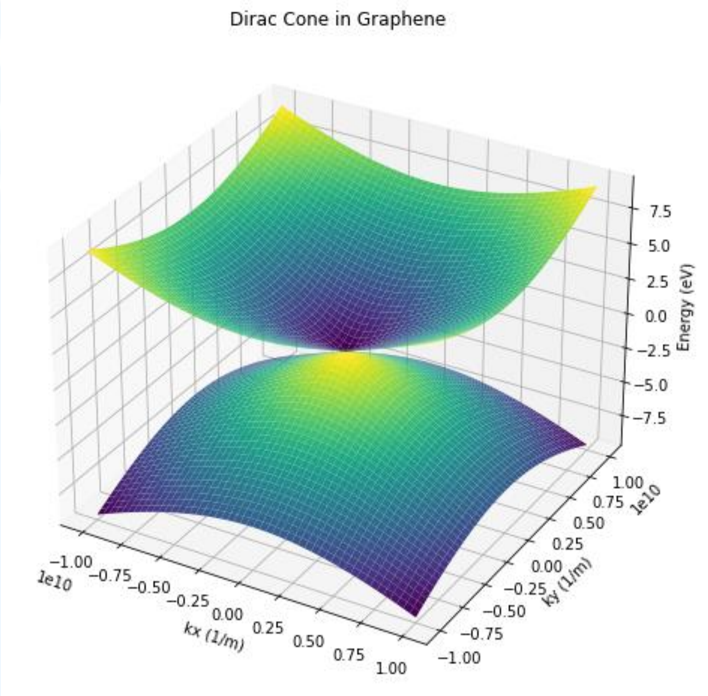
What is Graphene?

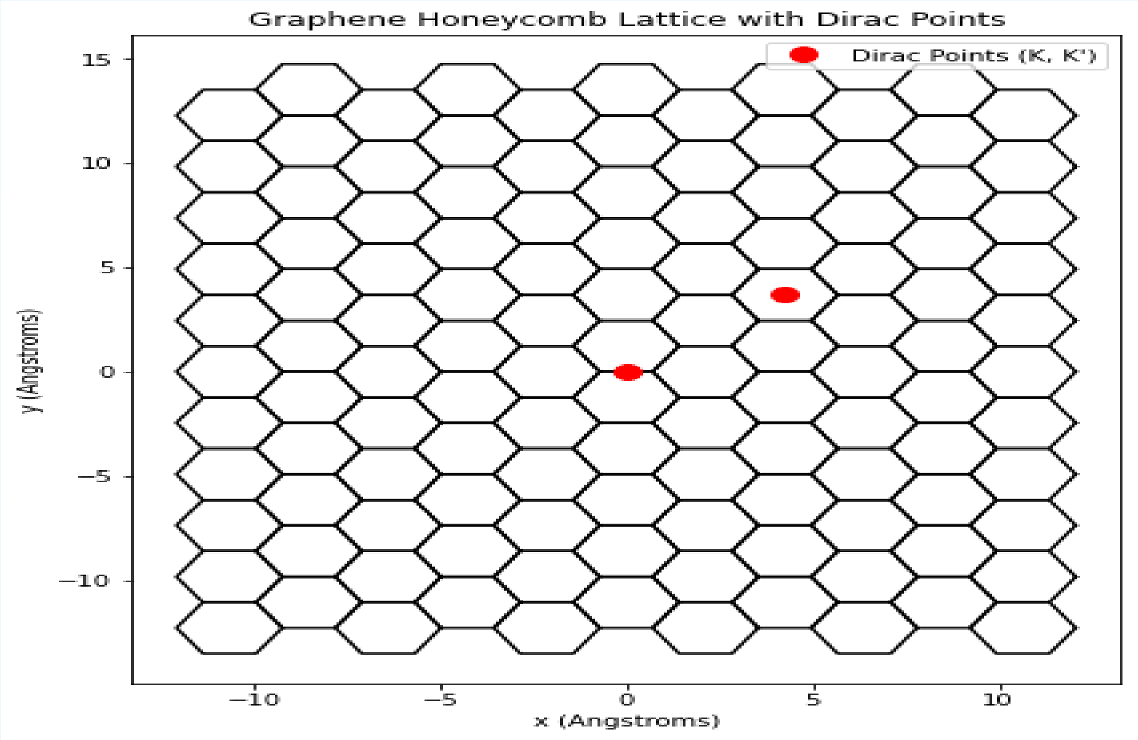
- A single layer of carbon atoms in a hexagonal lattice.
- Extraordinary properties: High electrical conductivity, strength, and optical transparency.

Relationship Between Graphene and the Dirac Equation

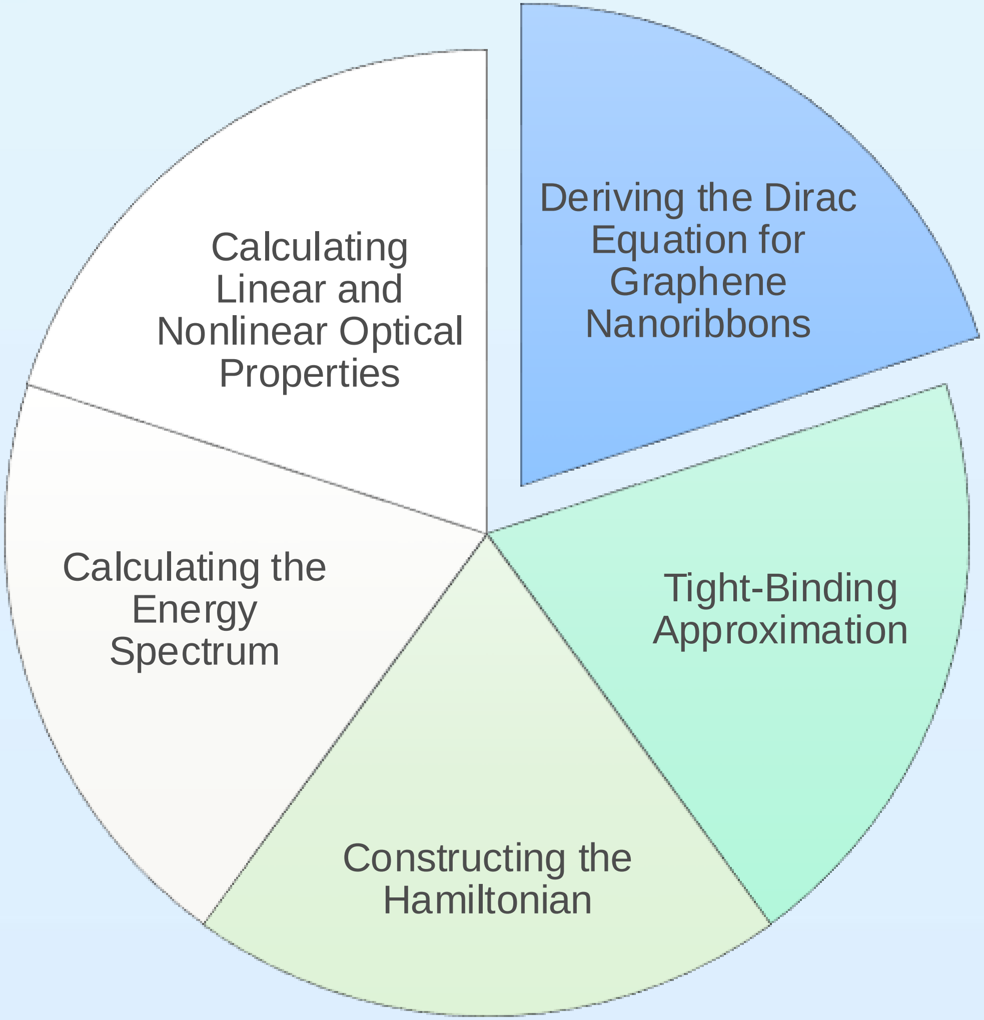
- In graphene, electrons behave like massless Dirac fermions.
- The electronic structure near the Dirac points in graphene is described by the Dirac equation.

Dirac cons Graphene





Methodology



Equations

- ✓ Dirac equation for 2D

$$v_F = (\sigma_x k_x + \sigma_y k_y)\psi = E\psi$$

- ✓ Boundary Conditions and Hamiltonian for Zigzag and Armchair Nanoribbons

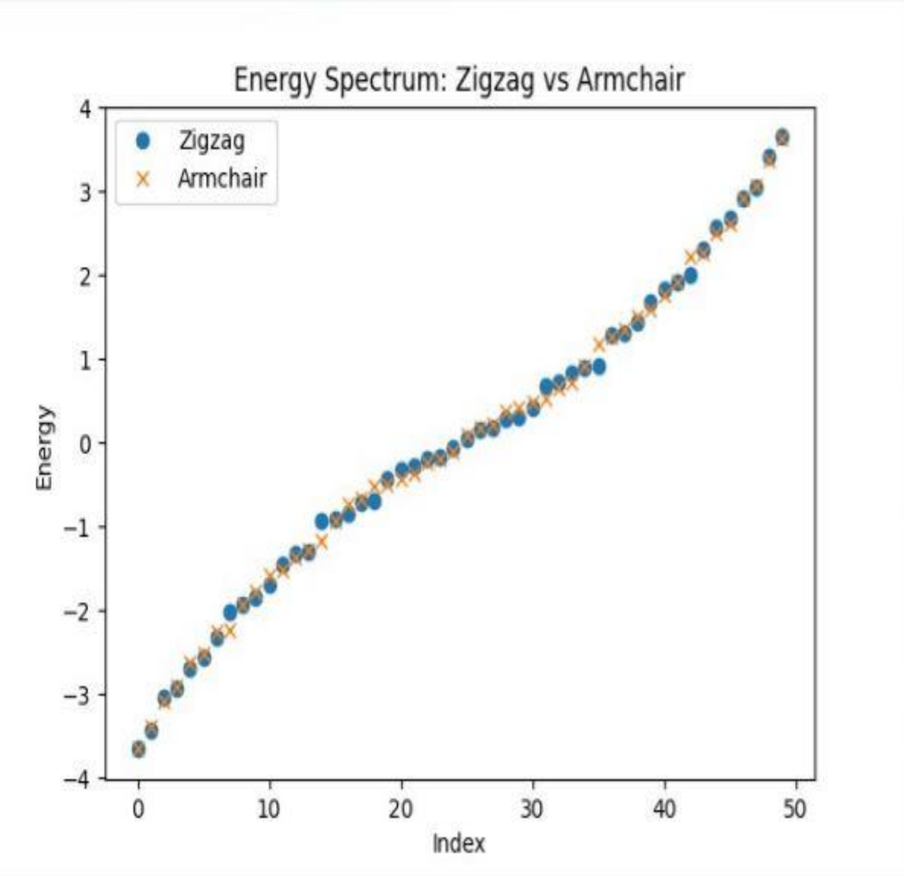
$$\psi(x=0) = \psi(x=L) = 0$$

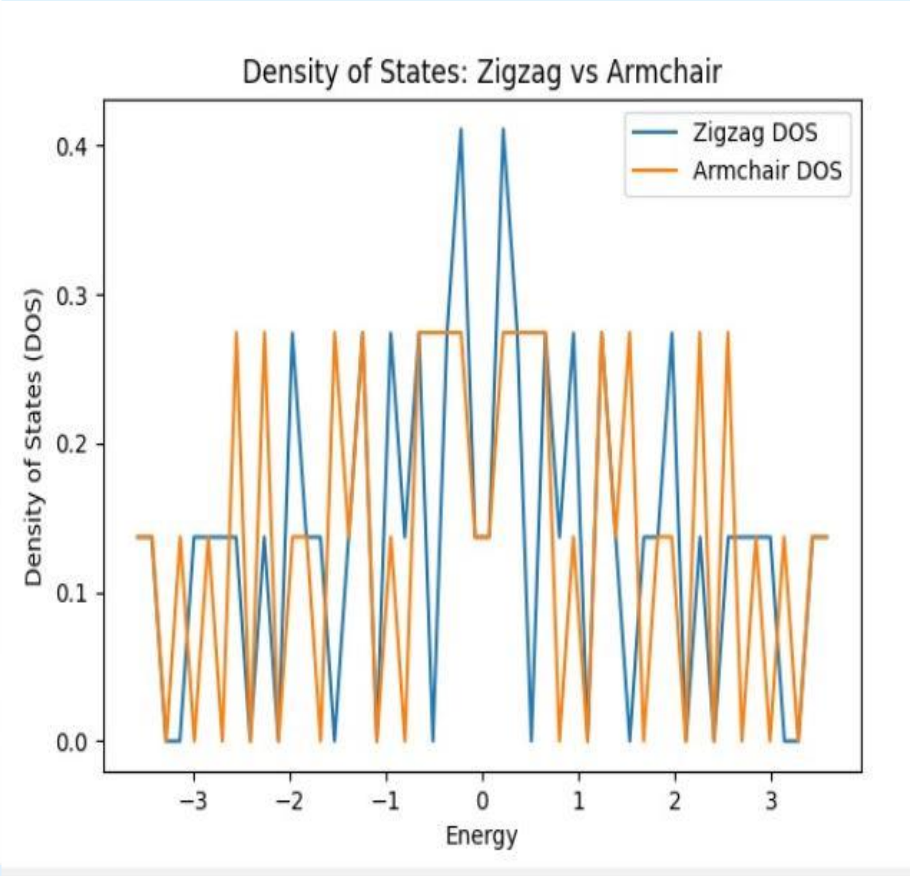
$$\psi_A(x=0) = \psi_A(x=L) = 0$$

$$\psi_B(x=0) = \psi_B(x=L) = 0$$

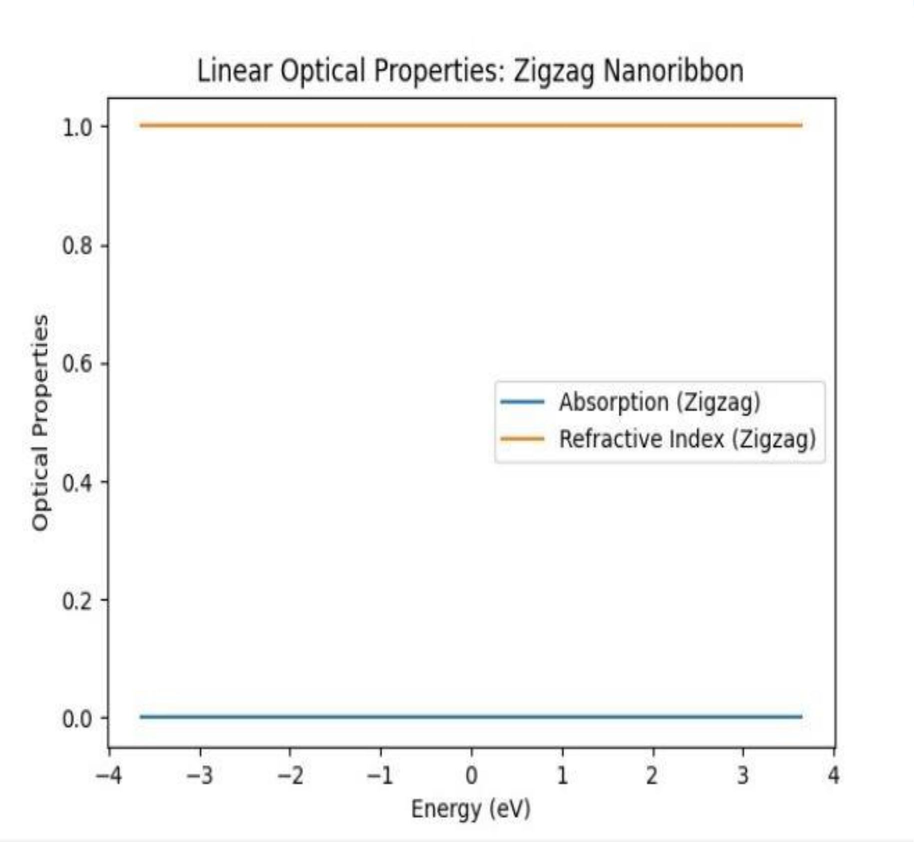
$$H = -t\sum_{\langle i,j\rangle}(c_i^{\dagger}c_j + hc)$$

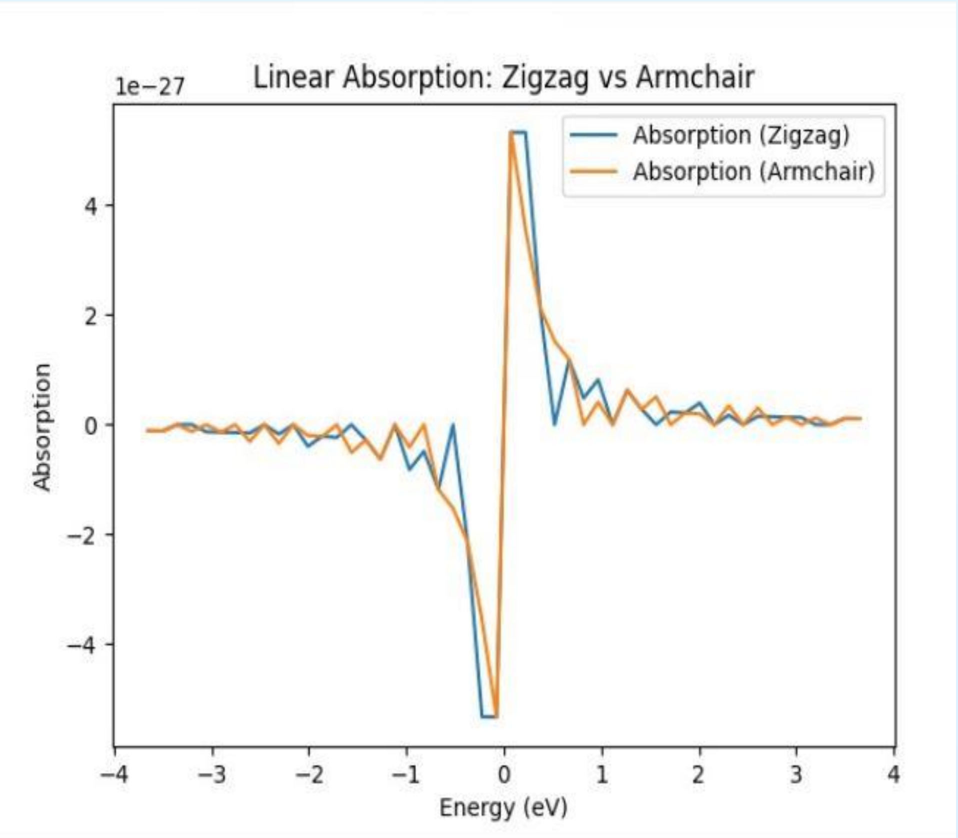
Density of state, energy spectrum



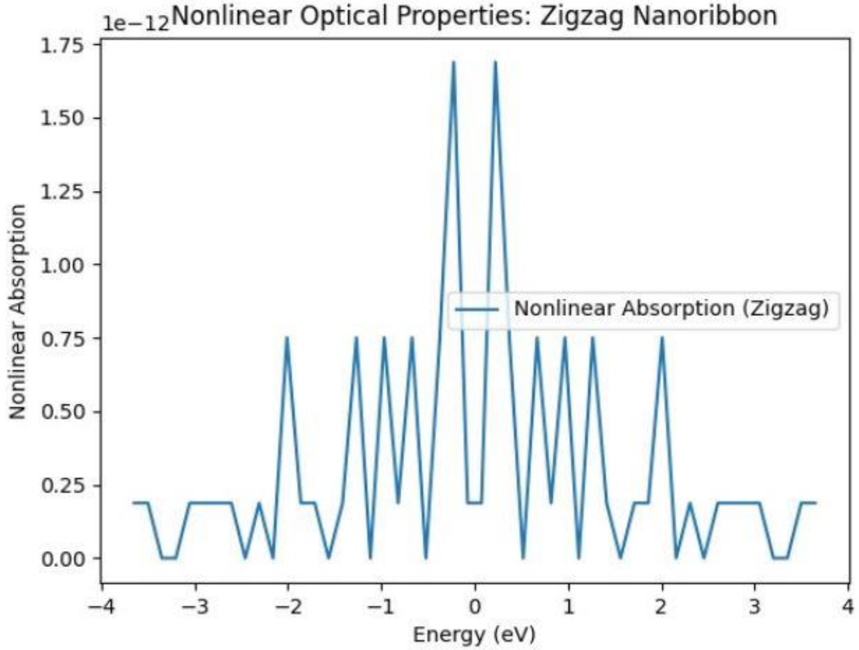


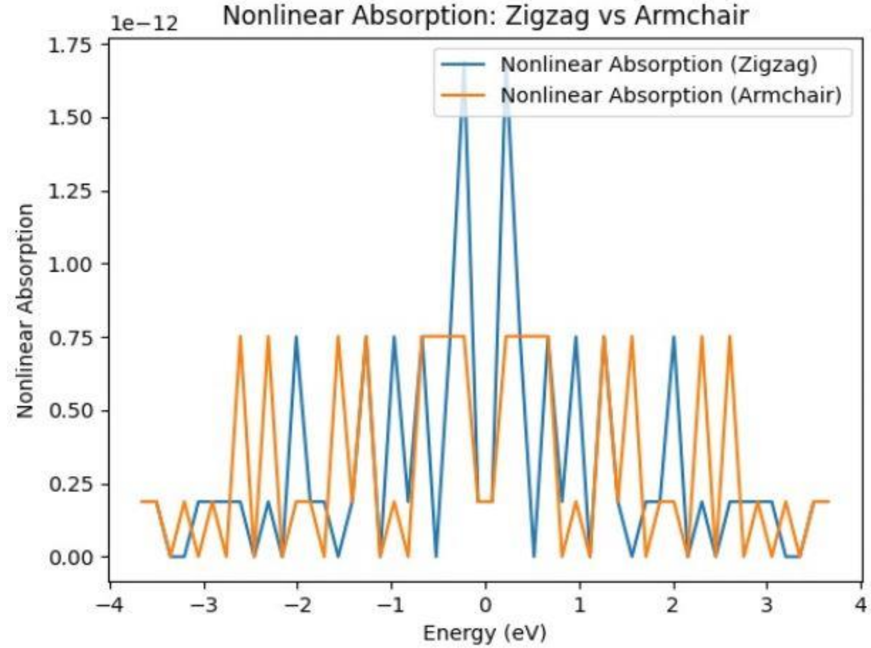
Liner Optical Properties





Non Liner Optical Properties





Thank you for your attention