Results of multilayers graphene under biaxial strain

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Introduction

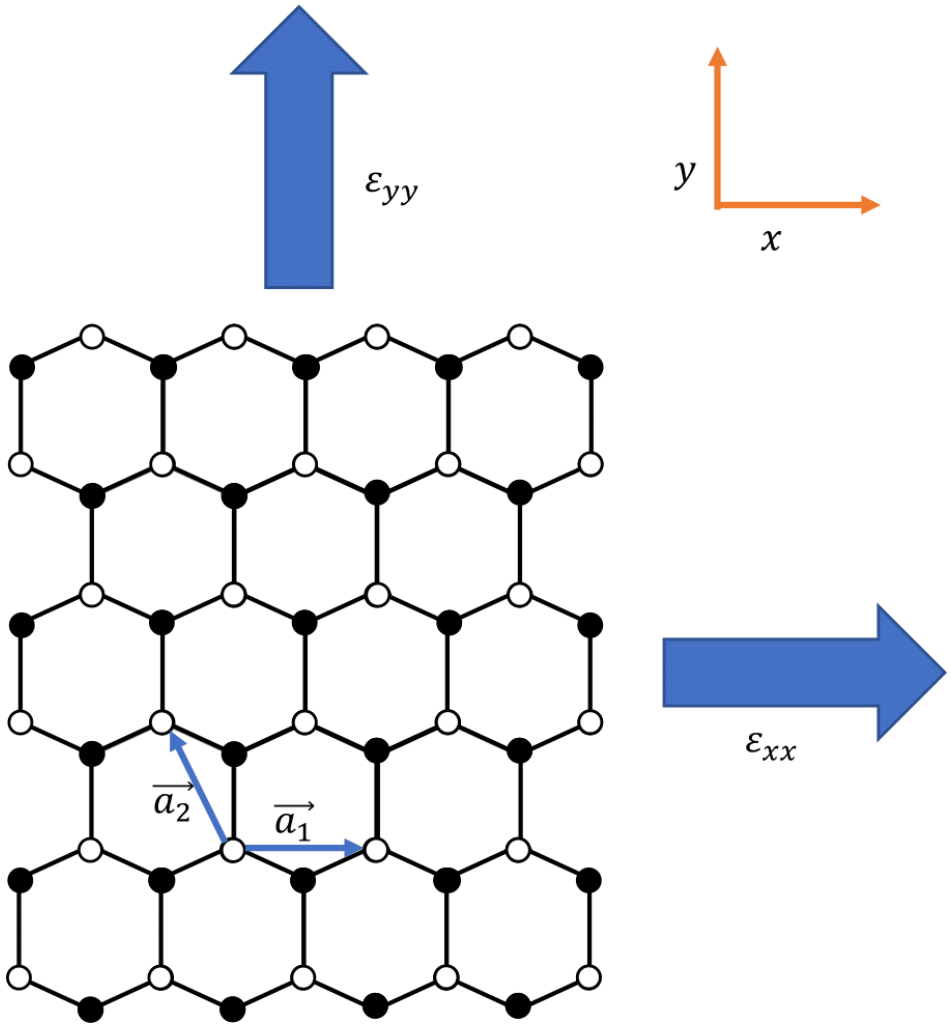


Figure: Illustration of the biaxial strain in the graphene

Monolayer graphene(PBE)

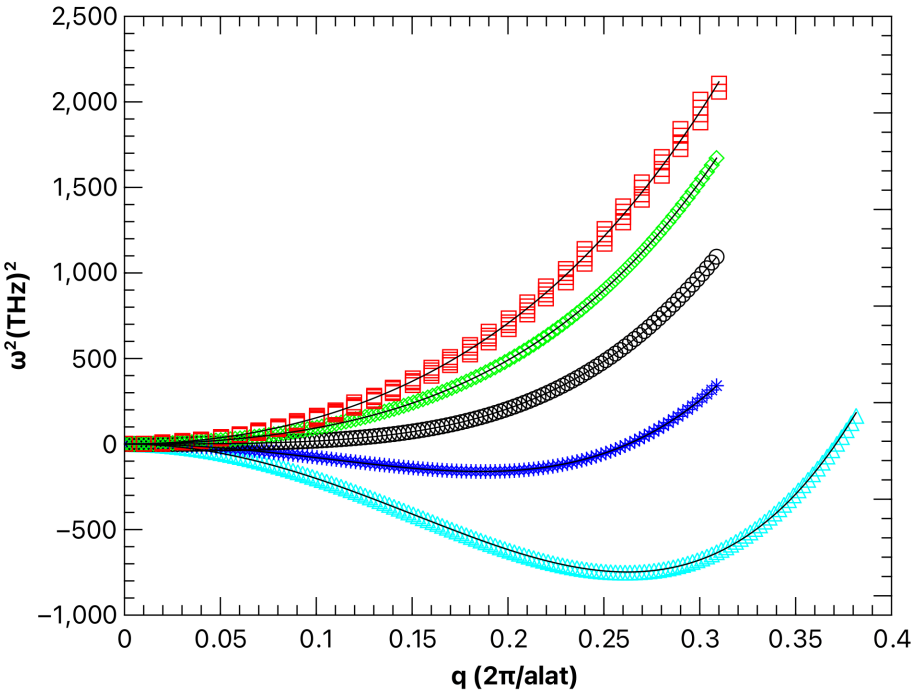
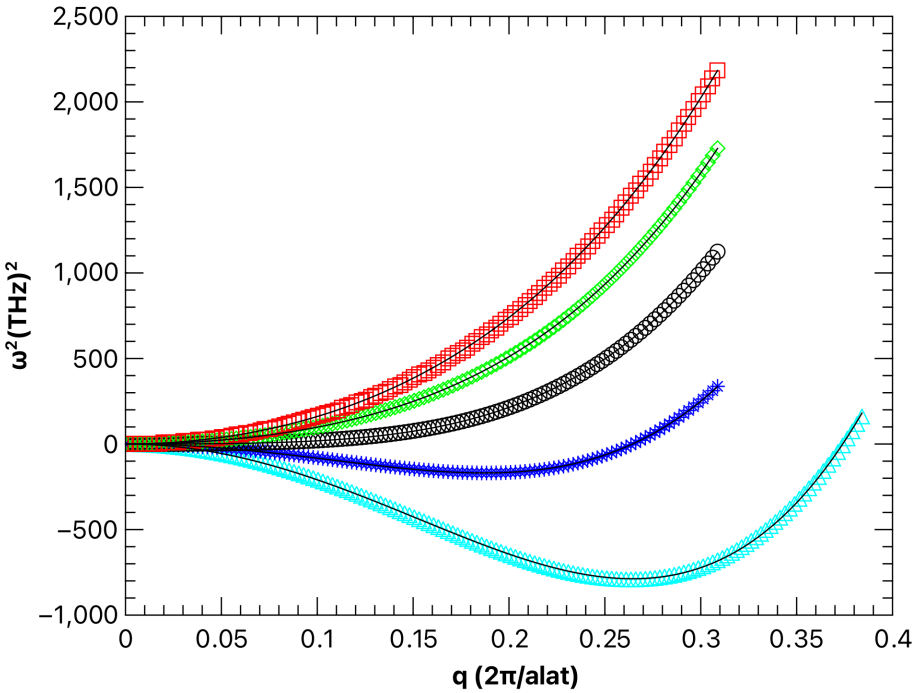


Figure: Low-quadratic frequency for graphene monolayer with LDA functional. Black circles: $\varepsilon = 0$. Diamond green: $\varepsilon = 2.5\%$. Red rectangle: $\varepsilon = 5\%$. Blue star: $\varepsilon = -2.5\%$. cyan triangle: $\varepsilon = -5\%$

Monolayer graphene(LDA)



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Bilayer graphene(LDA)

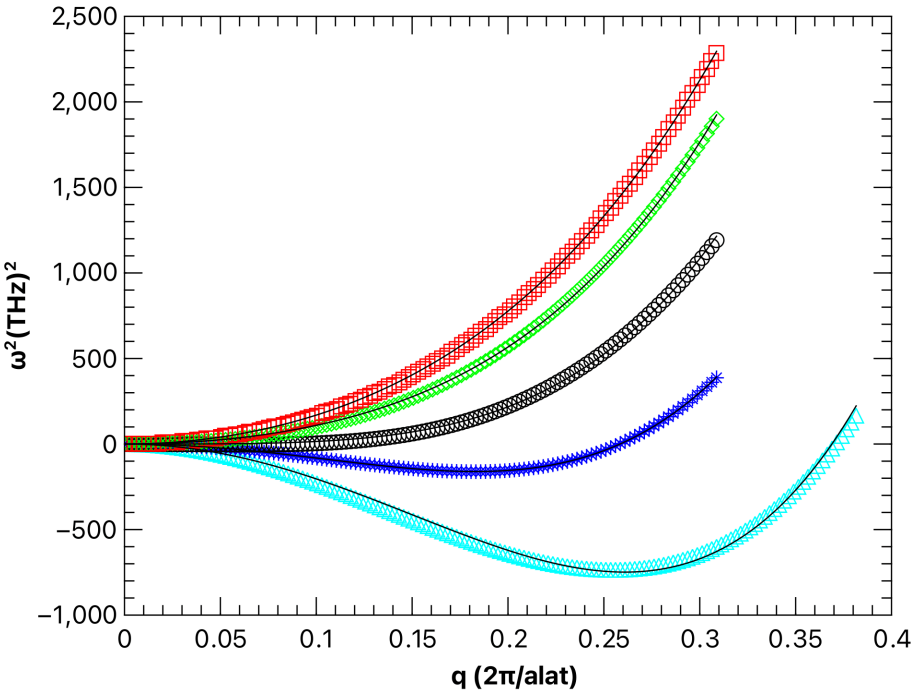

Figure: Low-quadratic frequency for graphene bilayer with LDA functional. Black circles: $\varepsilon = 0$. Diamond green: $\varepsilon = 2.5\%$. Red rectangle: $\varepsilon = 5\%$. Blue star: $\varepsilon = -2.5\%$. cyan triangle: $\varepsilon = -5\%$

Trilayer graphene(LDA)

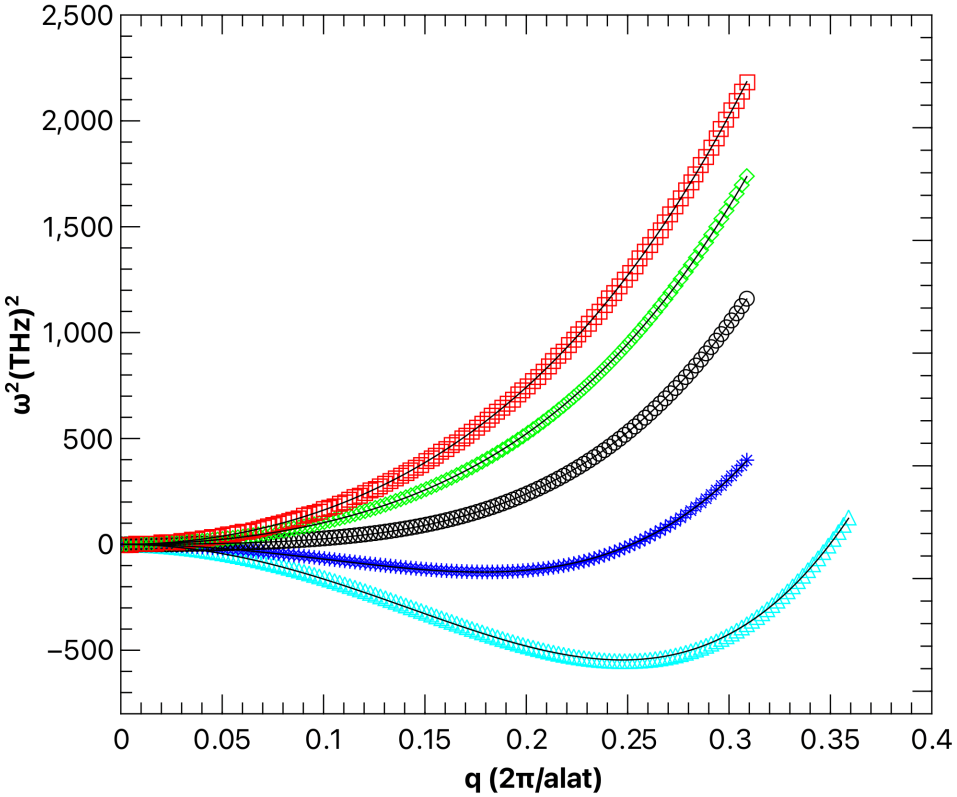

Figure: Low-quadratic frequency for graphene trilayer with LDA functional. Black circles: $\varepsilon = 0$. Diamond green: $\varepsilon = 2.5\%$. Red rectangle: $\varepsilon = 5\%$. Blue star: $\varepsilon = -2.5\%$. cyan triangle: $\varepsilon = -4.5\%$

Coefficient of linear term

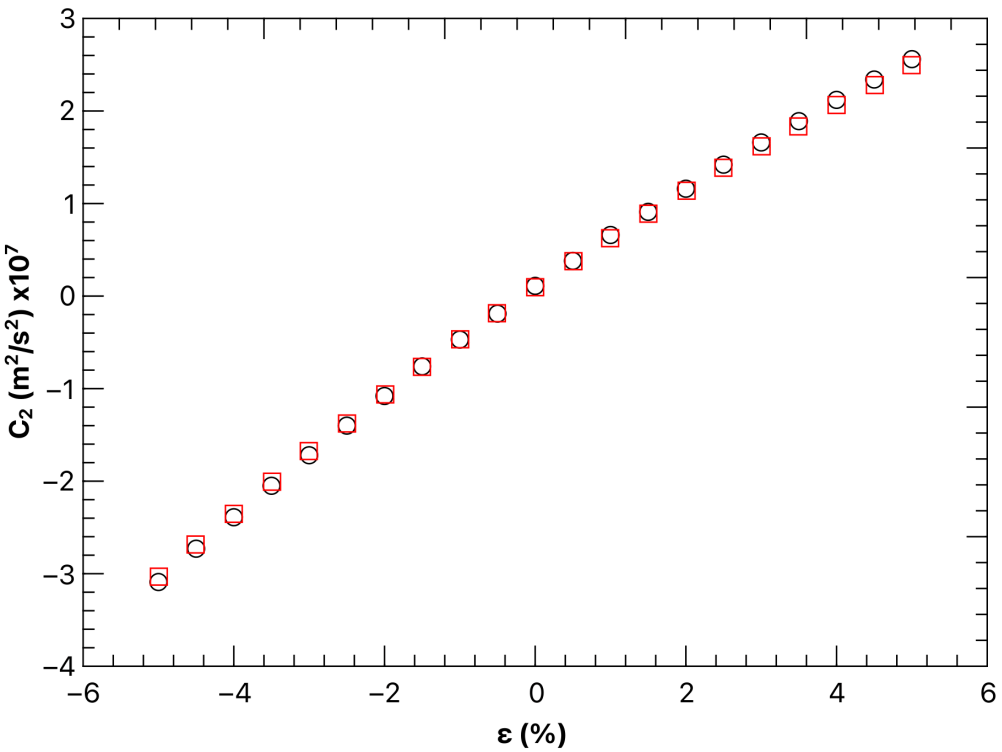

Figure: Coefficient of linear term for monolayer graphene for different values of strain. Black circles: LDA functional. Red rectangle: PBE functional.

Coefficient of linear term

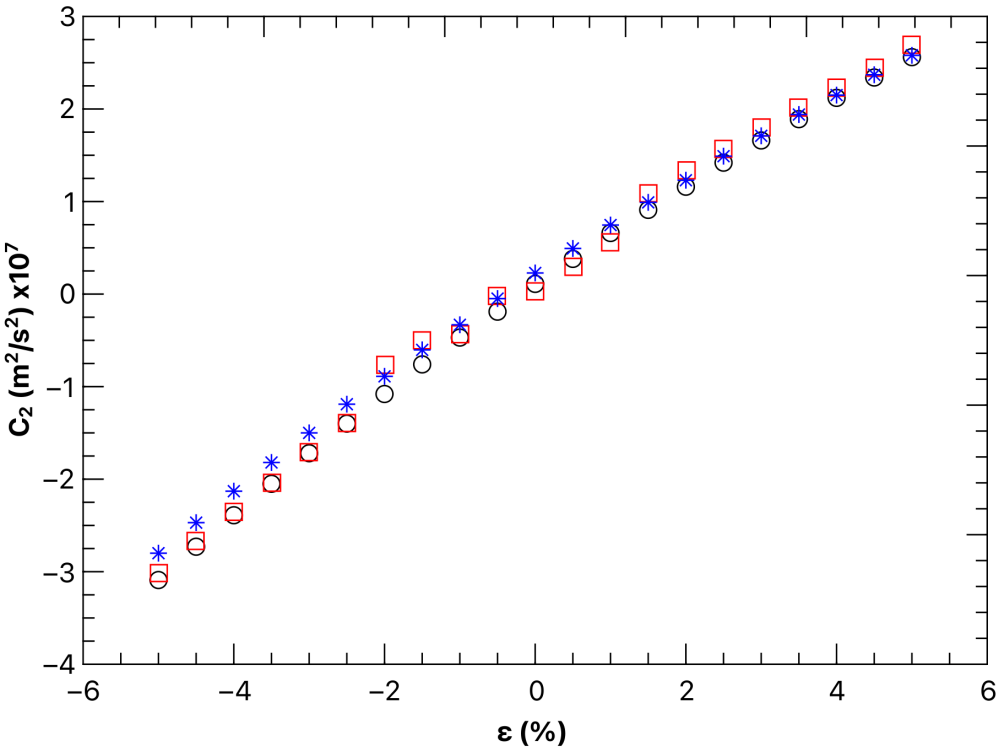

Figure: Coefficient of linear term for multilayers graphene for different values of strain with LDA functional. Black circles: Monolayer. Red rectangle: Bilayer. Blue star: Trilayer.

Coefficient of quadratic term

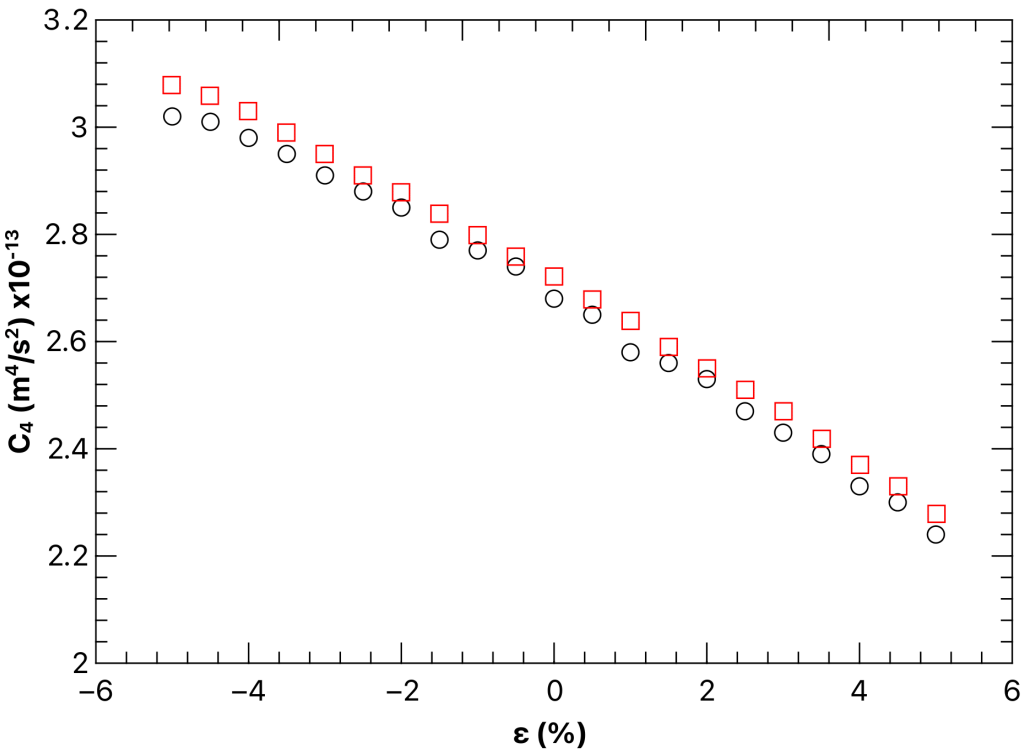

Figure: Coefficient of quadratic term for monolayer graphene for different values of strain. Black circles: LDA functional. Red rectangle: PBE functional.

Coefficient of quadratic term

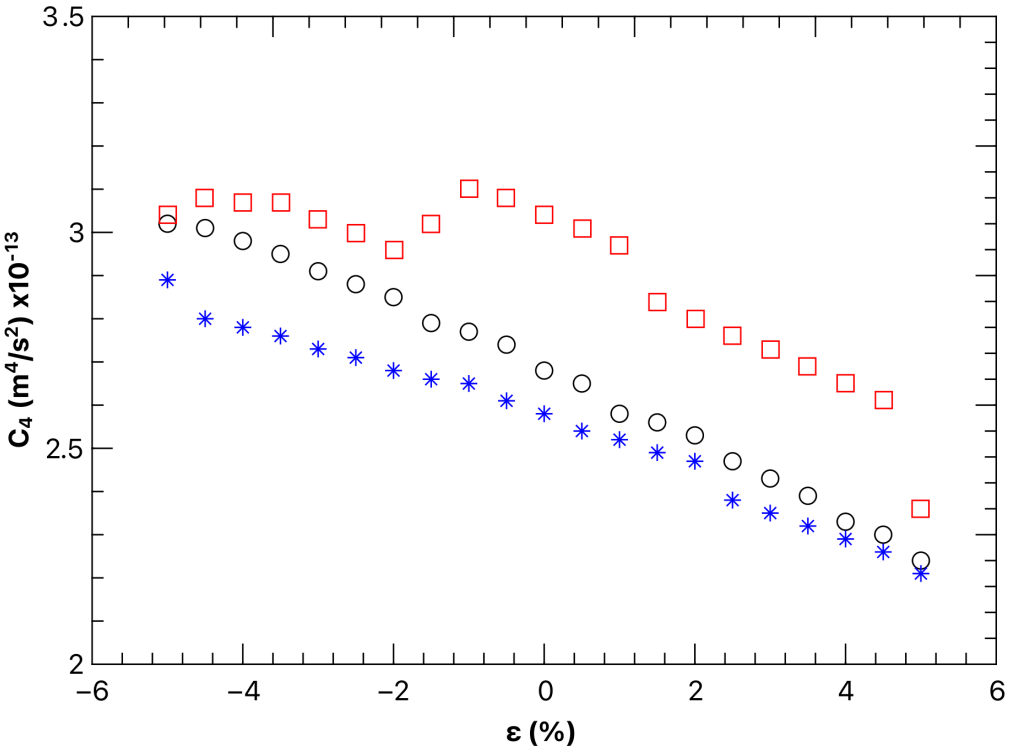

Figure: Coefficient of quadratic term for multilayers graphene for different values of strain with LDA functional. Black circles: Monolayer. Red rectangle: Bilayer. Blue star: Trilayer.

Critical value of q

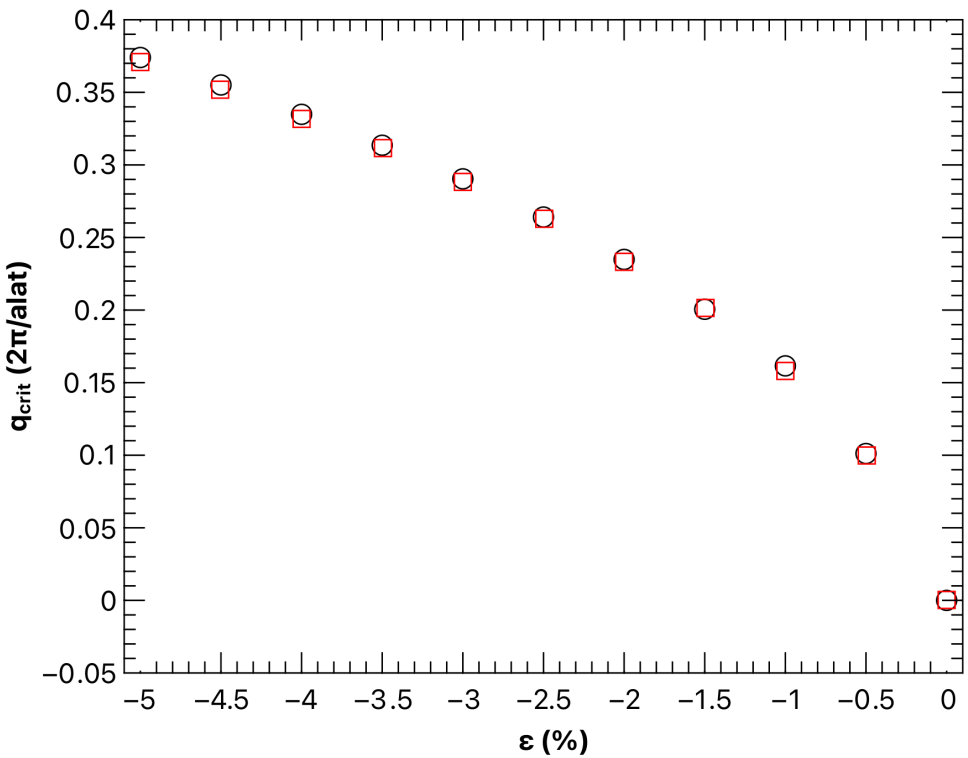

Figure: Critical value of q for monolayer graphene for different values of strain. Black circles: LDA functional. Red rectangle: PBE functional.

Critical value of q

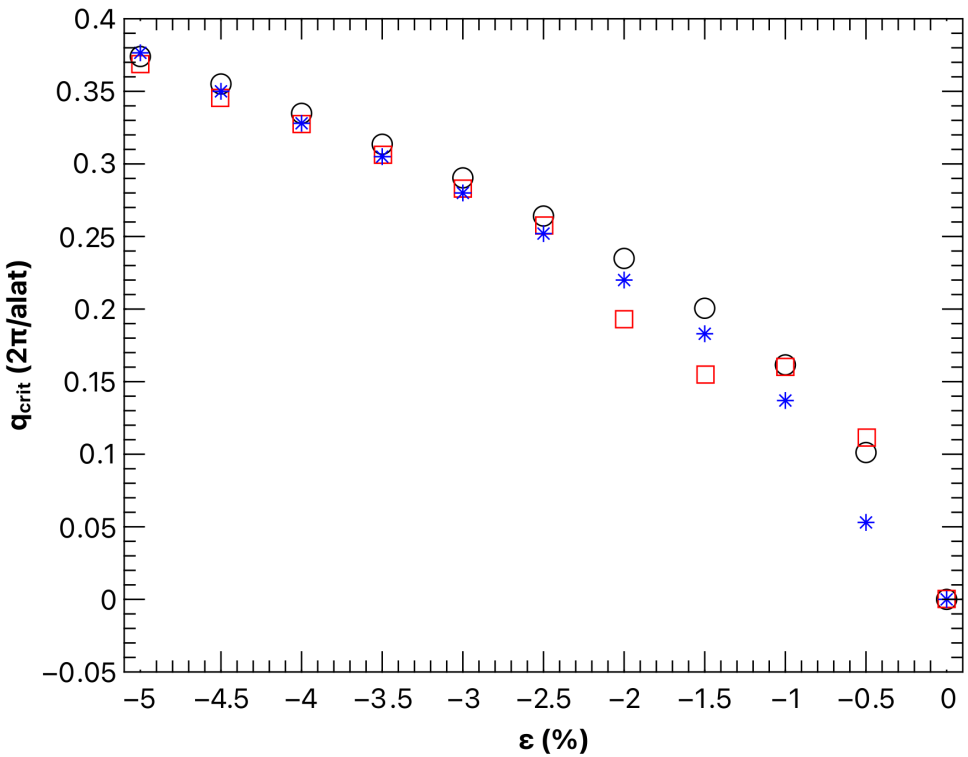

Figure: Critical value of q for multilayers graphene for different values of strain with LDA functional. Black circles: Monolayer. Red rectangle: Bilayer. Blue star: Trilayer.

Stress-strain

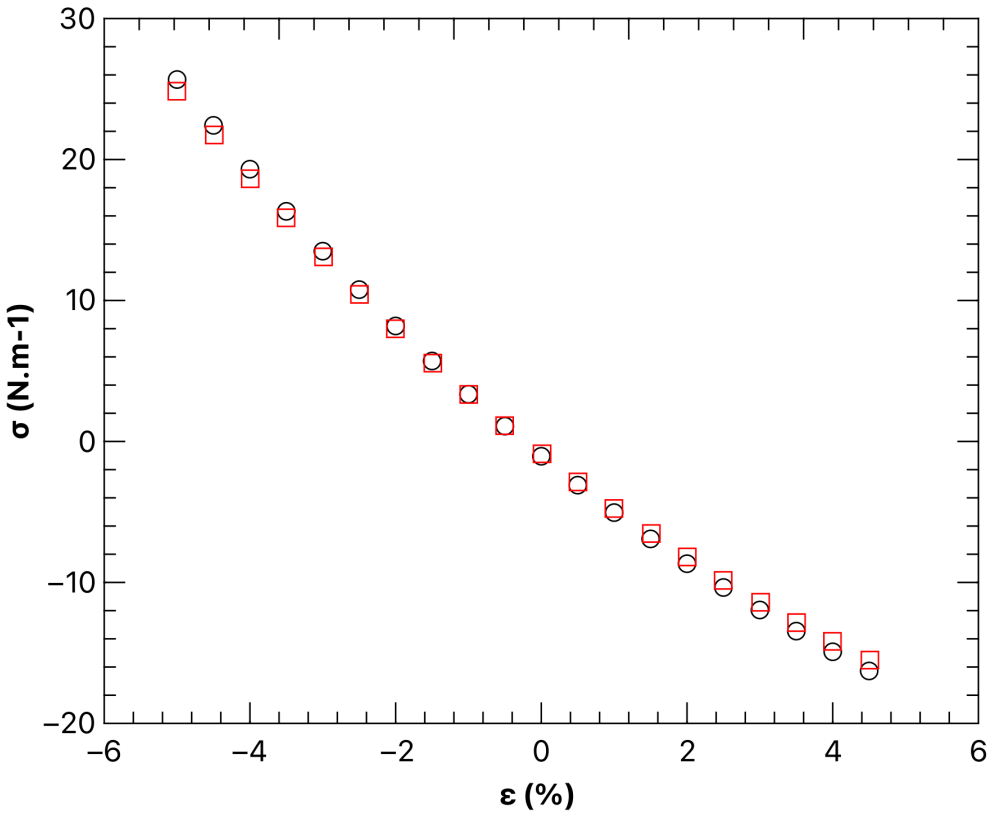

Figure: Stress for monolayer graphene for different values of strain. Black circles: LDA functional. Red rectangle: PBE functional.

Stress-strain

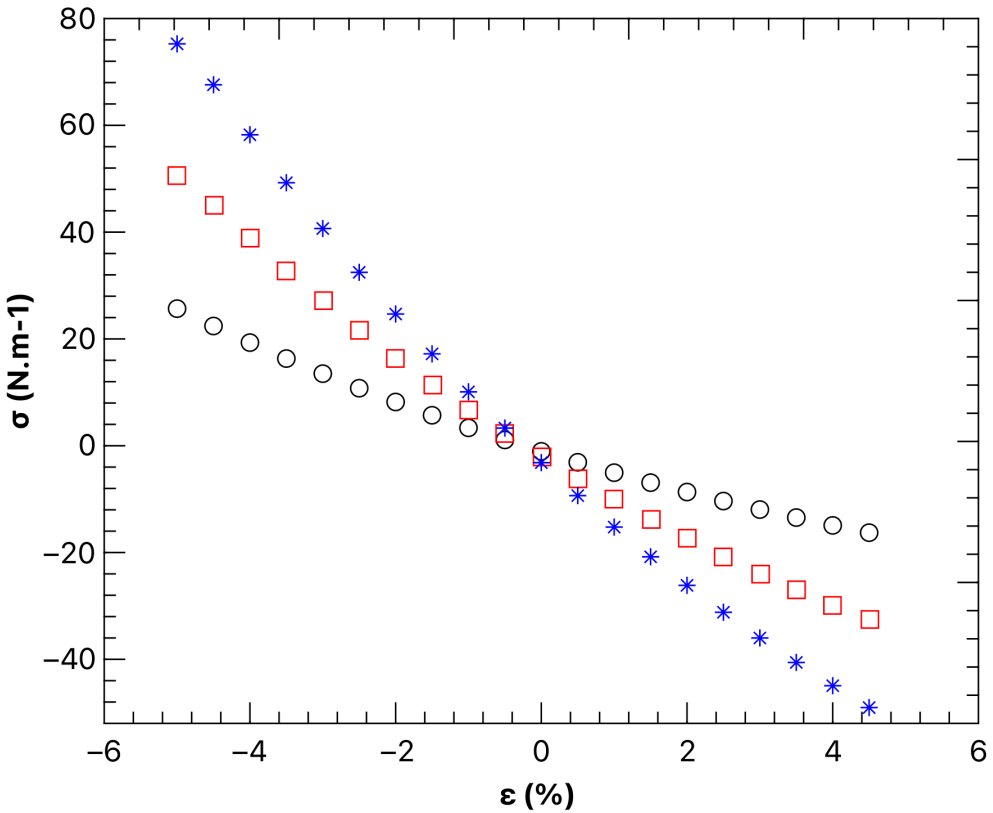

Figure: Stress for multilayers graphene for different values of strain with LDA functional. Black circles: Monolayer. Red rectangle: Bilayer. Blue star: Trilayer.

Bending rigidity

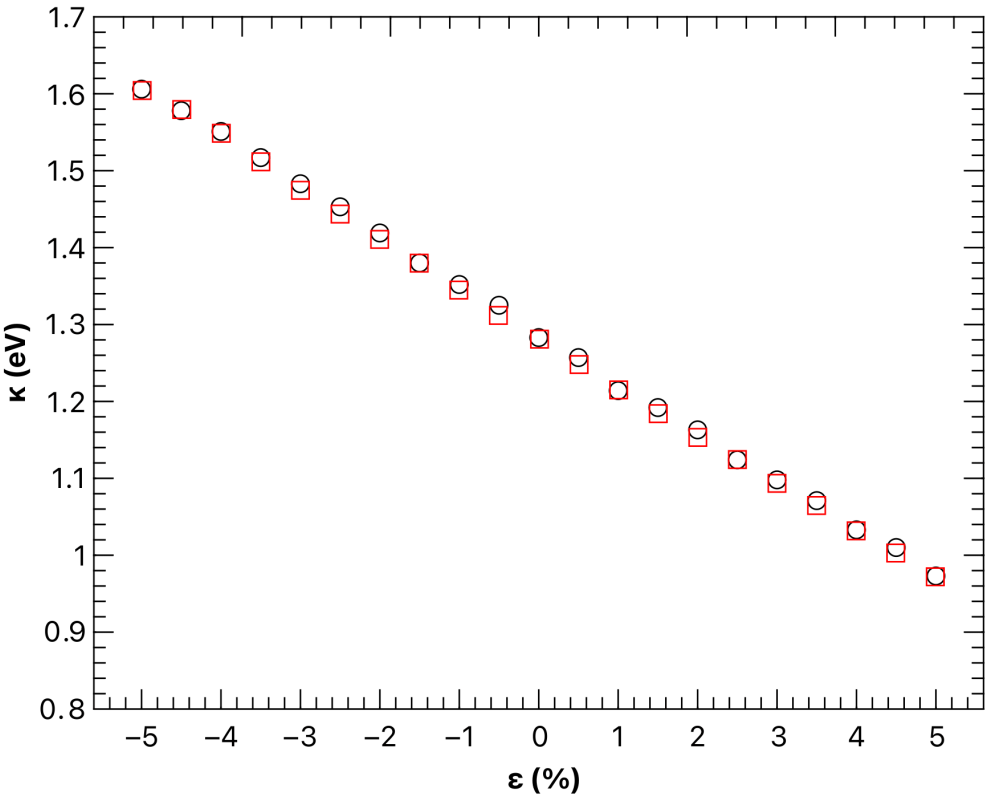

Figure: Bending rigidity for monolayer graphene for different values of strain. Black circles: LDA functional. Red rectangle: PBE functional.

Bending rigidity

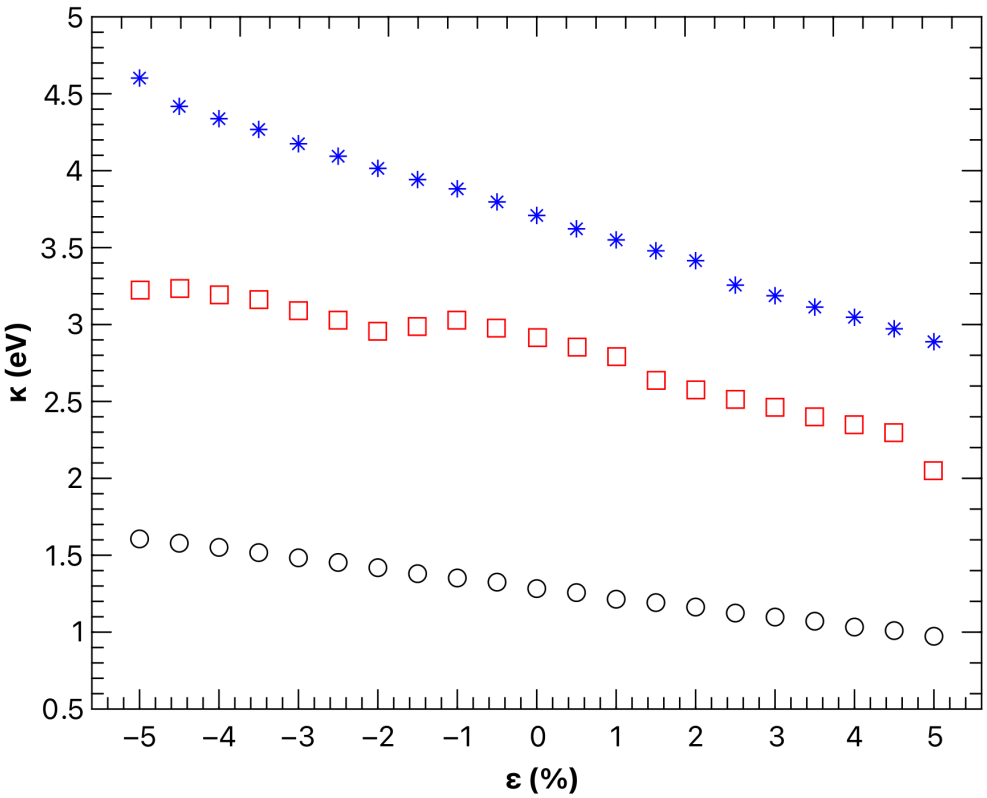

Figure: Bending rigidity for multilayers graphene for different values of strain with LDA functional. Black circles: Monolayer. Red rectangle: Bilayer. Blue star: Trilayer.

Continuum picture

Numerous researchers have studied the behavior of out-of plane mode (ZA) of graphene when $q \to 0$ with and without biaxial stress. We have two approaches to analyze our problem, the membrane model approach and the atomistic approach, among the continuum analyzes we have the model of [De Andres et al., 2012]:

$$\omega_{\mathbf{q}}^2 = \frac{\kappa}{\rho}\mathbf{q}^4 + \frac{2(\lambda+\mu)\bar{u}}{\rho}\mathbf{q}^2 \tag{1}$$

where $\bar{u} = \partial_x u_x = \partial_y u_y$. This model agrees with our results and predicts in a Good way the behavior of graphene under biaxial tension.

Atomistic picture

For the atomistic model we do not have a clear analytical model that predicts the behavior of graphene under biaxial deformation, but following the analysis of [Katsnelson, 2007], we obtain the model for the case of graphene without deformation:

$$\omega_{\mathbf{q}}^2 = \frac{\kappa}{\rho}\mathbf{q}^4 \tag{2}$$

Rotational invariance

From the work of [Katsnelson, 2007], we can see that Eq. 2 comes from a condition of rotational invariance:

$$\mathbf{u}_{nj} = \delta\boldsymbol{\omega} \times \mathbf{R}_{nj}^{(0)} \tag{3}$$

Where $\delta\boldsymbol{\omega}$ is the rotation angle. These rotations should not give rise to forces or torques acting on the atoms. we have

$$\sum_{nj} A_{0i,nj}^{zz} r_n^{\alpha} r_n^{\beta} = 0 \tag{4}$$

Where $\alpha, \beta = x, y$.

Rotational invariance

From [Jiang et al., 2015], we found the condition of the rigid rotational invariance which says that, if the system is rotated by $\mathbf{u}_i = \delta\boldsymbol{\omega} \times \mathbf{r}_i$, then we should have $\delta V = 0$as in the translational invariance condition. Where, the rotation angle is $|\delta\boldsymbol{\omega}|$ and the rotation direction is $\boldsymbol{\delta\omega}/|\boldsymbol{\delta\omega}|$.

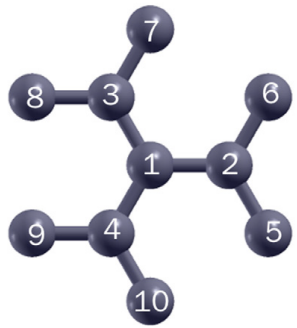

Figure: Sketch of the local environment of atom 1.

In this same work we found a expression for potential of the out-of-plane bond bending, this interaction is a four-body interaction. It describes the interaction between atom 1 and its neighboring atoms 2–4.

Rotational invariance

$$\mathbf{u}_i = \delta\boldsymbol{\omega} \times \mathbf{r}_i$$

For potential:

$$V_{rc} = \frac{k_{rc}}{2}\left[(3\mathbf{u}_1 - (\mathbf{u}_2 + \mathbf{u}_3 + \mathbf{u}_4)) \cdot \mathbf{e}^z\right]^2$$

$$V_{rc} = \frac{k_{rc}}{2}\left[((\mathbf{u}_1 - \mathbf{u}_2) + (\mathbf{u}_1 - \mathbf{u}_3) + (\mathbf{u}_1 - \mathbf{u}_4)) \cdot \mathbf{e}^z\right]^2$$

$$V_{rc} = \frac{k_{rc}}{2}\left[((\delta\boldsymbol{\omega} \times (\mathbf{r}_1 - \mathbf{r}_2)) + (\delta\boldsymbol{\omega} \times (\mathbf{r}_1 - \mathbf{r}_3)) + (\delta\boldsymbol{\omega} \times (\mathbf{r}_1 - \mathbf{r}_4))) \cdot \mathbf{e}^z\right]^2$$

$$V_{rc} = \frac{k_{rc}}{2}\left[((\delta\boldsymbol{\omega} \times \mathbf{r}_{21}) + (\delta\boldsymbol{\omega} \times \mathbf{r}_{31}) + (\delta\boldsymbol{\omega} \times \mathbf{r}_{41})) \cdot \mathbf{e}^z\right]^2$$

Rotational invariance

$$V_{rc} \approx \frac{k_{rc}}{2}\left[((\delta\boldsymbol{\omega} \times \mathbf{r}_{12}) + (\delta\boldsymbol{\omega} \times \mathbf{r}_{13}) + (\delta\boldsymbol{\omega} \times \mathbf{r}_{14})) \cdot \mathbf{e}^z\right]^2$$

$$V_{rc} \approx \frac{k_{rc}}{2}\left[(\delta\boldsymbol{\omega} \times (\mathbf{r}_{12} + \mathbf{r}_{13} + \mathbf{r}_{14})) \cdot \mathbf{e}^z\right]^2$$

For Rotational invariance:

$$V_{rc} \approx \frac{k_{rc}}{2}\left[(\delta\boldsymbol{\omega} \times (\mathbf{r}_{12} + \mathbf{r}_{13} + \mathbf{r}_{14})) \cdot \mathbf{e}^z\right]^2 = 0$$

For the rigid rotational invariance. It says that, if the system is rotated by $\mathbf{u}_i = \delta\boldsymbol{\omega} \times \mathbf{r}_i$, then we should also have $\delta V = 0$.

$$k_{rc}\left[(\delta\boldsymbol{\omega} \times (\mathbf{r}_{12} + \mathbf{r}_{13} + \mathbf{r}_{14})) \cdot \mathbf{e}^z\right]^2 = 0$$

Force constants

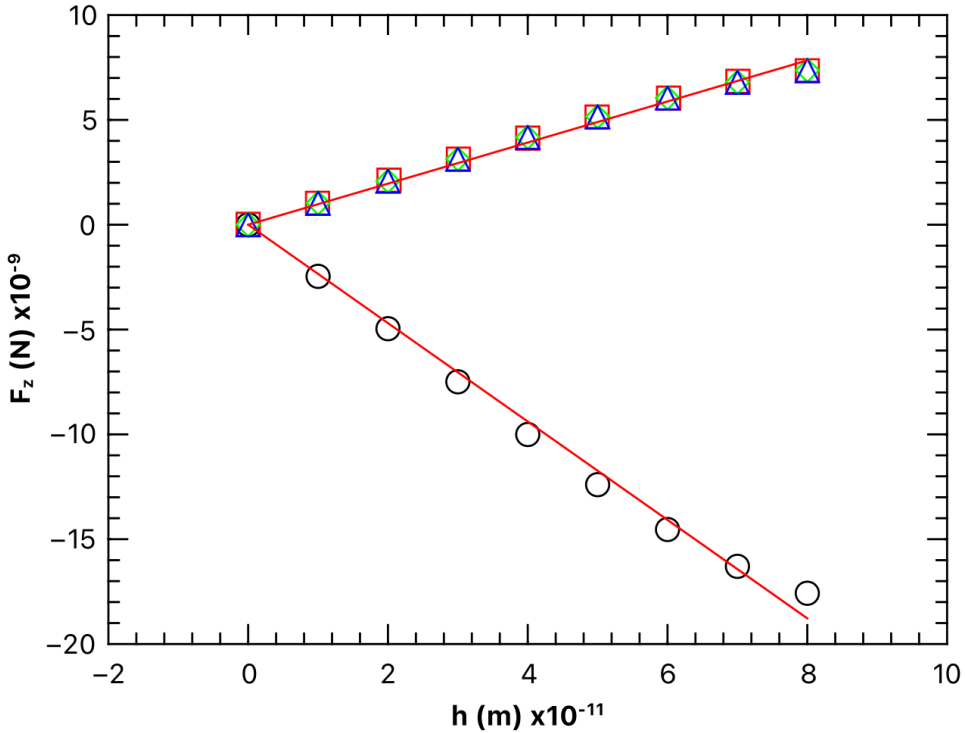

Figure: Force along z-axis of the first neighbors for different values of h of a supercell $8x8x1$ of graphene. Black circles: Atom 1. Red rectangle: Atom 2. Blue triangle: Atom 3.Green diamond: Atom 4

Force constants

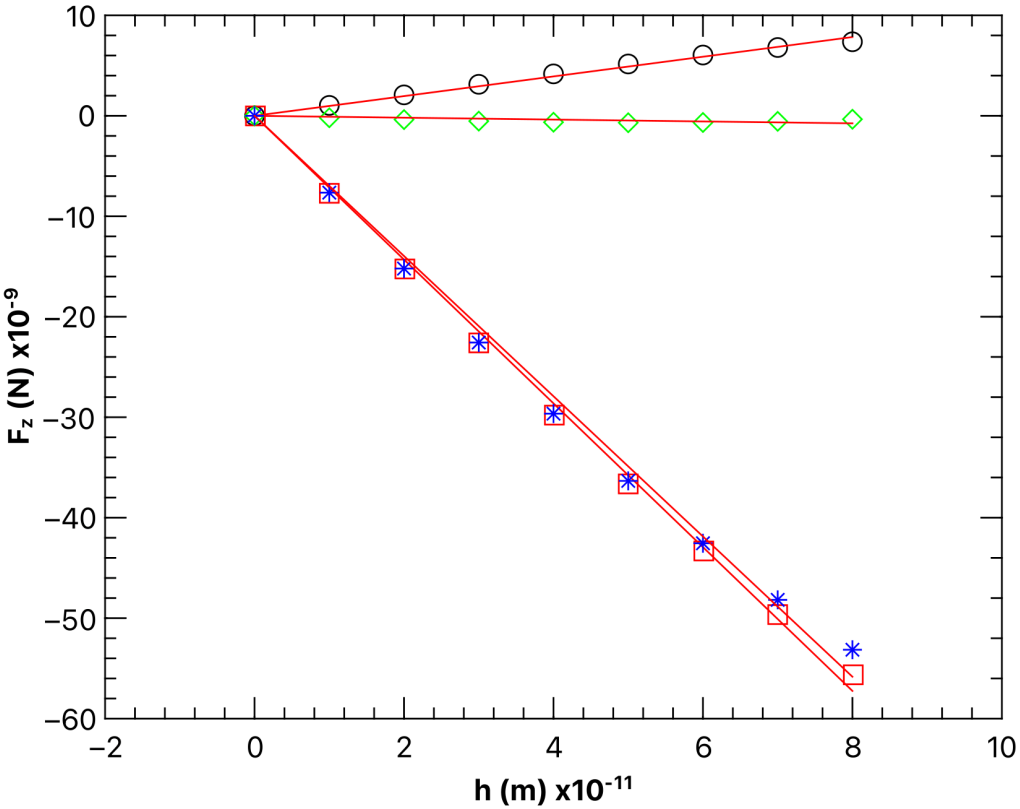

Figure: Force along z-axis of the first neighbors for different values of h of a supercell $8x8x1$ of graphene. Black circles: First Neighbors. Red rectangle: Second Neighbors . Blue star: Third neighbors. Green diamond: Fourth Neighbors

References


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