Supporting information

Raman spectra and corresponding strain effects in graphyne and graphdiyne

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1) Detailed process for deducing the frequency response functions linking small strain with the doubly degenerate E_{2g} Raman-active mode.

For a two-dimensional system under mechanical strain, a doubly degenerate mode splits into two bands. The energies of the splitting modes are the eigenvalues of the corresponding Hamiltonian:

$$\hat{H} = \begin{bmatrix} a & c \\ c & b \end{bmatrix} \tag{1}$$

where *a*, *b*, and *c* are matrix elements. The solutions of Eq. (1) are:

$$\omega_{1,2} = \frac{(a+b) \pm \sqrt{(a-b)^2 + 4c^2}}{2} \tag{2}$$

$a,\ b,$ and c under small strain can be expanded as:

$$\begin{cases} a = a_0 + \alpha_1\varepsilon_{xx} + \beta_1\varepsilon_{yy} + \chi_1\varepsilon_{xy} \\ b = b_0 + \alpha_2\varepsilon_{xx} + \beta_2\varepsilon_{yy} + \chi_2\varepsilon_{xy} \\ c = c_0 + \alpha_3\varepsilon_{xx} + \beta_3\varepsilon_{yy} + \chi_3\varepsilon_{xy} \end{cases} \tag{3}$$

The original state is degenerate, whose frequency is ω_0, so for an unstrained structure:

$$a = b, c = 0 \tag{4}$$

such that $a_0 = b_0 = \omega_0, c_0 = 0$. Under strain, the split frequencies can be written as

$$\omega_{1,2} = a_0 + \frac{(\alpha_1+\alpha_2)\varepsilon_{xx} + (\beta_1+\beta_2)\varepsilon_{yy} + (\chi_1+\chi_2)\varepsilon_{xy}}{2} \pm \frac{\sqrt{[(\alpha_1-\alpha_2)\varepsilon_{xx} + (\beta_1-\beta_2)\varepsilon_{yy} + (\chi_1-\chi_2)\varepsilon_{xy}]^2 + 4(\alpha_3\varepsilon_{xx} + \beta_3\varepsilon_{yy} + \chi_3\varepsilon_{xy})^2}}{2} \tag{5}$$

Then, we will solve the relationships of the whole coefficients by symmetry restrictions of the D_{6h} point group.

(1) Inversion operation: If changing the sign of shear strain ($\varepsilon_{xy} \rightarrow -\varepsilon_{xy}$) in Eq. (5), the frequencies are invariant.

$$\omega_{1,2} = a_0 + \frac{(\alpha_1+\alpha_2)\varepsilon_{xx} + (\beta_1+\beta_2)\varepsilon_{yy} + (\chi_1+\chi_2)\varepsilon_{xy}}{2}$$
$$\pm \frac{\sqrt{[(\alpha_1-\alpha_2)\varepsilon_{xx} + (\beta_1-\beta_2)\varepsilon_{yy} + (\chi_1-\chi_2)\varepsilon_{xy}]^2 + 4(\alpha_3\varepsilon_{xx} + \beta_3\varepsilon_{yy} + \chi_3\varepsilon_{xy})^2}}{2}$$
$$\equiv a_0 + \frac{(\alpha_1+\alpha_2)\varepsilon_{xx} + (\beta_1+\beta_2)\varepsilon_{yy} - (\chi_1+\chi_2)\varepsilon_{xy}}{2}$$
$$\pm \frac{\sqrt{[(\alpha_1-\alpha_2)\varepsilon_{xx} + (\beta_1-\beta_2)\varepsilon_{yy} - (\chi_1-\chi_2)\varepsilon_{xy}]^2 + 4(\alpha_3\varepsilon_{xx} + \beta_3\varepsilon_{yy} - \chi_3\varepsilon_{xy})^2}}{2} \tag{6}$$

Thus, we have

$$\begin{cases} \chi_1 + \chi_2 = 0 \\ (\alpha_1-\alpha_2)(\chi_1-\chi_2) + 4\alpha_3\chi_3 = 0 \\ (\beta_1-\beta_2)(\chi_1-\chi_2) + 4\beta_3\chi_3 = 0 \end{cases} \tag{7}$$

(2) To apply equivalent uniaxial strain along the x and y directions ($\varepsilon_{xx} = \varepsilon_{yy} = \varepsilon, \varepsilon_{xy} = 0$), the symmetry is conserved, and no split happens. Thus,

$$\frac{\sqrt{[(\alpha_1-\alpha_2)\varepsilon + (\beta_1-\beta_2)\varepsilon]^2 + 4(\alpha_3\varepsilon + \beta_3\varepsilon)^2}}{2} \equiv 0$$

such that

$$\begin{cases} \alpha_1 + \beta_1 = \alpha_2 + \beta_2 \\ \alpha_3 + \beta_3 = 0 \end{cases} \tag{8}$$

(3) The system is invariable after a 60-degree rotation. The rotation of a second-rank tensor is given generally as

$$\begin{bmatrix} \varepsilon'_{xx} & \varepsilon'_{xy} \\ \varepsilon'_{xy} & \varepsilon'_{yy} \end{bmatrix} = \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} \varepsilon_{xx} & \varepsilon_{xy} \\ \varepsilon_{xy} & \varepsilon_{yy} \end{bmatrix} \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$$
$$= \begin{bmatrix} \varepsilon_{xx}\cos^2\theta + \varepsilon_{yy}\sin^2\theta + 2\varepsilon_{xy}\sin\theta\cos\theta & \varepsilon_{xy}(\cos^2\theta - \sin^2\theta) - (\varepsilon_{xx}-\varepsilon_{yy})\sin\theta\cos\theta \\ \varepsilon_{xy}(\cos^2\theta - \sin^2\theta) - (\varepsilon_{xx}-\varepsilon_{yy})\sin\theta\cos\theta & \varepsilon_{xx}\sin^2\theta + \varepsilon_{yy}\cos^2\theta - 2\varepsilon_{xy}\sin\theta\cos\theta \end{bmatrix} \tag{9}$$

When $\theta = \frac{\pi}{3}$, the strain tensor becomes:

$$\begin{bmatrix} \frac{1}{4}\varepsilon_{xx} + \frac{3}{4}\varepsilon_{yy} + \frac{\sqrt{3}}{2}\varepsilon_{xy} & \frac{1}{2}\varepsilon_{xy} - \frac{\sqrt{3}}{4}(\varepsilon_{xx}-\varepsilon_{yy}) \\ \frac{1}{2}\varepsilon_{xy} - \frac{\sqrt{3}}{4}(\varepsilon_{xx}-\varepsilon_{yy}) & \frac{3}{4}\varepsilon_{xx} + \frac{1}{4}\varepsilon_{yy} - \frac{\sqrt{3}}{2}\varepsilon_{xy} \end{bmatrix} \tag{10}$$

Thus, we have:

$$\omega_{1,2} = a_0 + \frac{(\alpha_1+\alpha_2)\varepsilon_{xx} + (\beta_1+\beta_2)\varepsilon_{yy} + (\chi_1+\chi_2)\varepsilon_{xy}}{2} \pm \frac{\sqrt{[(\alpha_1-\alpha_2)\varepsilon_{xx} + (\beta_1-\beta_2)\varepsilon_{yy} + (\chi_1-\chi_2)\varepsilon_{xy}]^2 + 4(\alpha_3\varepsilon_{xx} + \beta_3\varepsilon_{yy} + \chi_3\varepsilon_{xy})^2}}{2}$$

$$\equiv a_0 + \frac{(\alpha_1+\alpha_2)\left(\frac{1}{4}\varepsilon_{xx} + \frac{3}{4}\varepsilon_{yy} + \frac{\sqrt{3}}{2}\varepsilon_{xy}\right) + (\beta_1+\beta_2)\left(\frac{3}{4}\varepsilon_{xx} + \frac{1}{4}\varepsilon_{yy} - \frac{\sqrt{3}}{2}\varepsilon_{xy}\right) - (\chi_1+\chi_2)\left[\frac{1}{2}\varepsilon_{xy} - \frac{\sqrt{3}}{4}(\varepsilon_{xx}-\varepsilon_{yy})\right]}{2}$$

$$\pm \frac{\sqrt{\begin{array}{c}\left\{(\alpha_1-\alpha_2)\left(\frac{1}{4}\varepsilon_{xx} + \frac{3}{4}\varepsilon_{yy} + \frac{\sqrt{3}}{2}\varepsilon_{xy}\right) + (\beta_1-\beta_2)\left(\frac{3}{4}\varepsilon_{xx} + \frac{1}{4}\varepsilon_{yy} - \frac{\sqrt{3}}{2}\varepsilon_{xy}\right) + (\chi_1-\chi_2)\left[\frac{1}{2}\varepsilon_{xy} - \frac{\sqrt{3}}{4}(\varepsilon_{xx}-\varepsilon_{yy})\right]\right\}^2 \\ +4\alpha_3\left(\frac{1}{4}\varepsilon_{xx} + \frac{3}{4}\varepsilon_{yy} + \frac{\sqrt{3}}{2}\varepsilon_{xy}\right) + \beta_3\left(\frac{3}{4}\varepsilon_{xx} + \frac{1}{4}\varepsilon_{yy} - \frac{\sqrt{3}}{2}\varepsilon_{xy}\right) - \chi_3\left[\frac{1}{2}\varepsilon_{xy} - \frac{\sqrt{3}}{4}(\varepsilon_{xx}-\varepsilon_{yy})\right]^2\end{array}}}{2} \tag{11}$$

The equality of the first term in Eq. (11) gives:

$$\begin{cases} (\alpha_1+\alpha_2) = \frac{1}{4}(\alpha_1+\alpha_2) + \frac{3}{4}(\beta_1+\beta_2) - \frac{\sqrt{3}}{4}(\chi_1+\chi_2) \\ (\beta_1+\beta_2) = \frac{3}{4}(\alpha_1+\alpha_2) + \frac{1}{4}(\beta_1+\beta_2) + \frac{\sqrt{3}}{4}(\chi_1+\chi_2) \\ (\chi_1+\chi_2) = \frac{\sqrt{3}}{2}(\alpha_1+\alpha_2) - \frac{\sqrt{3}}{2}(\beta_1+\beta_2) + \frac{1}{2}(\chi_1+\chi_2) \end{cases} \tag{12}$$

Combining with Eq. (7), we have:

$$(\alpha_1+\alpha_2) = (\beta_1+\beta_2) \tag{13}$$

Based on Eqs. (7, 8, 13), combined with the definitions $\bar{\alpha} = \frac{\alpha_1+\alpha_2}{2} = \frac{\beta_1+\beta_2}{2}$, $\Delta\alpha = \frac{\alpha_1-\alpha_2}{2} = \frac{\beta_1-\beta_2}{2}$, we have:

$$\begin{cases} \alpha_1 = \bar{\alpha} - \Delta\alpha \\ \alpha_2 = \bar{\alpha} + \Delta\alpha \\ \beta_1 = \bar{\alpha} + \Delta\alpha \\ \beta_2 = \bar{\alpha} - \Delta\alpha \\ \beta_3 = -\alpha_3 \\ \chi_2 = -\chi_1 \\ \chi_3 = \frac{\Delta\alpha\chi_1}{\alpha_3} \end{cases} \tag{14}$$

Eq. (14) reduces the number of coefficients from 9 to 4.

The equality of the second term in Eq. (11) gives:

$$
\begin{aligned}
&[(\alpha_1-\alpha_2)\varepsilon_{xx}+(\beta_1-\beta_2)\varepsilon_{yy}+(\chi_1-\chi_2)\varepsilon_{xy}]^2+4(\alpha_3\varepsilon_{xx}+\beta_3\varepsilon_{yy}+\chi_3\varepsilon_{xy})^2\\
&\equiv\left\{\left[\frac{1}{4}(\alpha_1-\alpha_2)+\frac{3}{4}(\beta_1-\beta_2)-\frac{\sqrt{3}}{4}(\chi_1-\chi_2)\right]\varepsilon_{xx}\right.\\
&+\left[\frac{3}{4}(\alpha_1-\alpha_2)+\frac{1}{4}(\beta_1-\beta_2)+\frac{\sqrt{3}}{4}(\chi_1-\chi_2)\right]\varepsilon_{yy}\\
&\left.+\left[\frac{\sqrt{3}}{2}(\alpha_1-\alpha_2-\beta_1+\beta_2)+\frac{1}{2}(\chi_1-\chi_2)\right]\varepsilon_{xy}\right\}^2\\
&+4\left\{\left(\frac{1}{4}\alpha_3+\frac{3}{4}\beta_3-\frac{\sqrt{3}}{4}\chi_3\right)\varepsilon_{xx}+\left(\frac{3}{4}\alpha_3+\frac{1}{4}\beta_3+\frac{\sqrt{3}}{4}\chi_3\right)\varepsilon_{yy}\right.\\
&\left.+\left[\frac{\sqrt{3}}{2}(\alpha_3-\beta_3)+\frac{1}{2}\chi_3\right]\varepsilon_{xy}\right\}^2
\end{aligned}
\tag{15}
$$

Combined with Eq. (14), Eq. (15) reduces to:

$$
\begin{aligned}
&\left(-2\Delta\alpha\varepsilon_{xx}+2\Delta\alpha\varepsilon_{yy}+2\chi_1\varepsilon_{xy}\right)^2+4\left(\alpha_3\varepsilon_{xx}-\alpha_3\varepsilon_{yy}+\frac{\Delta\alpha\chi_1}{\alpha_3}\varepsilon_{xy}\right)^2\\
&\equiv\left\{\left[\frac{1}{2}\Delta\alpha+\frac{3}{2}\Delta\alpha-\frac{\sqrt{3}}{2}\chi_1\right]\varepsilon_{xx}+\left[-\frac{3}{2}\Delta\alpha+\frac{1}{2}\Delta\alpha+\frac{\sqrt{3}}{2}\chi_1\right]\varepsilon_{yy}+\left(2\sqrt{3}\Delta\alpha+\chi_1\right)\varepsilon_{xy}\right\}^2\\
&+4\left[\left(\frac{1}{4}\alpha_3-\frac{3}{4}\alpha_3-\frac{\sqrt{3}}{4}\frac{\Delta\alpha\chi_1}{\alpha_3}\right)\varepsilon_{xx}+\left(\frac{3}{4}\alpha_3-\frac{1}{4}\alpha_3+\frac{\sqrt{3}}{4}\frac{\Delta\alpha\chi_1}{\alpha_3}\right)\varepsilon_{yy}\right.\\
&\left.+\left(\sqrt{3}\alpha_3+\frac{1}{2}\frac{\Delta\alpha\chi_1}{\alpha_3}\right)\varepsilon_{xy}\right]^2
\end{aligned}
\tag{16}
$$

It is equivalent to

$$
\begin{aligned}
&\left[-2\Delta\alpha\left(\varepsilon_{xx}-\varepsilon_{yy}\right)+2\chi_1\varepsilon_{xy}\right]^2+4\left(\alpha_3\left(\varepsilon_{xx}-\varepsilon_{yy}\right)+\frac{\Delta\alpha\chi_1}{\alpha_3}\varepsilon_{xy}\right)^2\\
&\equiv\left[\left(\Delta\alpha-\frac{\sqrt{3}}{2}\chi_1\right)\left(\varepsilon_{xx}-\varepsilon_{yy}\right)+\left(2\sqrt{3}\Delta\alpha+\chi_1\right)\varepsilon_{xy}\right]^2\\
&+4\left[\left(-\frac{1}{2}\alpha_3-\frac{\sqrt{3}}{4}\frac{\Delta\alpha\chi_1}{\alpha_3}\right)\left(\varepsilon_{xx}-\varepsilon_{yy}\right)+\left(\sqrt{3}\alpha_3+\frac{1}{2}\frac{\Delta\alpha\chi_1}{\alpha_3}\right)\varepsilon_{xy}\right]^2
\end{aligned}
$$

(17)

Both sides whose corresponding terms are equal, so we have:

$$\begin{cases} 4(\Delta\alpha)^2 + 4\alpha_3^2 = \left(\Delta\alpha - \frac{\sqrt{3}}{2}\chi_1\right)^2 + 4\left(\frac{1}{2}\alpha_3 + \frac{\sqrt{3}}{4}\frac{\Delta\alpha\chi_1}{\alpha_3}\right)^2 \\ 4\chi_1^2 + 4\left(\frac{\Delta\alpha\chi_1}{\alpha_3}\right)^2 = \left(2\sqrt{3}\Delta\alpha + \chi_1\right)^2 + 4\left(\sqrt{3}\alpha_3 + \frac{1}{2}\frac{\Delta\alpha\chi_1}{\alpha_3}\right)^2 \\ -4\Delta\alpha\chi_1 + 4\alpha_3\frac{\Delta\alpha\chi_1}{\alpha_3} = 0 = \left(\Delta\alpha - \frac{\sqrt{3}}{2}\chi_1\right)\left(2\sqrt{3}\Delta\alpha + \chi_1\right) - 4\left(\frac{1}{2}\alpha_3 + \frac{\sqrt{3}}{4}\frac{\Delta\alpha\chi_1}{\alpha_3}\right)\left(\sqrt{3}\alpha_3 + \frac{1}{2}\frac{\Delta\alpha\chi_1}{\alpha_3}\right) \end{cases}$$

(18)

The definition $\chi_3 = \frac{\Delta\alpha\chi_1}{\alpha_3}$ is meaningless at $\chi_1 = \alpha_3 = 0$. If we regard χ_3 as an independent parameter, one solution of Eq. (17) is:

$$\begin{cases} \chi_1 = \alpha_3 = 0 \\ \chi_3 = \frac{\Delta\alpha\chi_1}{\alpha_3} = \pm 2\Delta\alpha \end{cases}$$

(19)

If we plug these relationships from Eqs. (14, 19) into the eigenvalue Eq. (5), the split frequencies of degenerate mode will be:

$$\omega_{1,2} = \omega_0 + \bar{\alpha}(\varepsilon_{xx} + \varepsilon_{yy}) \pm \Delta\alpha\sqrt{(\varepsilon_{xx} - \varepsilon_{yy})^2 + 4\varepsilon_{xy}^2}$$

(20)

This gives a universal formulation linking strain and the frequencies of the split doubly degenerate modes.

2) The response curves of Raman frequencies with uniaxial and shear strains

Let us return to the evolutions of Raman shifts with uniaxial strain and shear strain in graphene, graphyne (GY), and graphdiyne (GDY), which are presented in Figure 5. The response curves of Raman frequencies to strains are fitted by quadratic functions; generally, they can be expressed as $\omega = \mathrm{B2} \times \varepsilon^2 + \mathrm{B1} \times \varepsilon + \mathrm{B0}$, where $\mathrm{B0}, \mathrm{B1}$, and $\mathrm{B2}$ are the intercept, monomial, and quadratic coefficients, respectively, and the ratio between B2 and B1 ($\mathrm{B2/B1}$) can reflect the relative contribution of nonlinear effects to some extent; ε is the applied strain; and ω is the corresponding frequency. Most often, when the applied strain is small, the frequency can be assumed to be linearly associated with the strain. Inevitably there are still some nonlinear effects, which are unified into quadratic terms. The detailed values of B1 and B2 are presented in Tables S1 and S2. However, the B2 values are much smaller than the B1 values, so the most important contributors in this system are the linear terms. The $\mathrm{B2/B1}$ ratios under shear strain are generally greater than under uniaxial strain, which means the nonlinear effects by shear strain are more obvious than uniaxial strain. There are two possible reasons for these effects: one is the variations of structures under shear strain are stronger, another reason maybe attribute to the nonlinearly transition from structure to frequency. Thus, under uniaxial strain, we consider the strain from -4% to +4%, but under shear strain, where the strain was restrainted to [−3%, +3%] to reduce errors by nonlinear effects.

Table S1. Response curves coefficients linking frequencies with uniaxial strain

		B1 (cm^{-1}/%)	B2 (cm^{-1}/%^{2})	B2/B1
graphene	G_x^+	−23.8	0.37	−0.015
	G_x^-	−36.8	0.26	−0.007
	G_y^+	−22.9	0.27	−0.011
	G_y^-	−36.2	0.12	−0.003
GY	B_x	−26.8	0.15	−0.006
	B_y	−26.3	0.17	−0.006
	G_x^+	−26.8	0.21	−0.008
	G_x^-	−30.7	0.42	−0.014
	G_y^+	−26.3	0.42	−0.016
	G_y^-	−30.5	0.74	−0.024
	Y_x	−30.2	−1.97	0.065
	Y_y	−26.2	−1.79	0.068
GDY	B_x	−20.0	0.16	−0.008
	B_y	−19.8	0.16	−0.008
	G''^+_x	−23.4	0.08	−0.003
	G''^-_x	−34.3	−1.39	0.040
	G''^+_y	−24.6	0.78	−0.032
	G''^-_y	−33.2	0.68	−0.020
	G'_x	−35.6	−0.87	0.024
	G'_y	−33.4	−0.48	0.014
	G_x^+	−25.8	0.37	−0.014
	G_x^-	−38.5	1.87	−0.049
	G_y^+	−26.3	2.23	−0.085
	G_y^-	−39.9	0.33	−0.008
	Y_x	−35.1	−2.18	0.062
	Y_y	−30.8	−2.09	0.068
	Y'^+_x	−23.0	0.13	−0.006
	Y'^-_x	−44.0	2.79	−0.063
	Y'^+_y	−25.3	2.49	−0.098

Y'^{-}_{y}	−45.9	0.20	−0.004

Table S2. Response curves coefficients linking frequencies with shear strain

		B1 (cm^{-1}/%)	B2 (cm^{-1}/%^{2})	B2/B1
graphene	G_+	−3.08	−3.21	1.042
	G_-	6.16	2.73	0.443
GY	B	−0.30	0.57	−1.900
	G_+	−4.50	−1.01	0.224
	G_-	1.51	−0.23	−0.152
	Y	−11.8	−4.12	0.349
GDY	B	1.29	0.00	0.000
	G''_+	−9.41	−3.48	0.370
	G''_-	10.8	−3.24	−0.300
	G'	−5.52	−1.6	0.290
	G_+	−9.49	0.96	−0.101
	G_-	16.5	2.83	0.172
	Y	−8.3	−6.48	0.781
	Y'_+	−18.2	2.42	−0.133
	Y'_-	27.6	1.58	0.057

3) Variations of bond lengths and angles versus uniaxial strain and shear strain

Figures S1 and S2 show the variations in bond lengths and angles with uniaxial strain and shear strain, respectively. The structures of graphene, GY, and GDY are shown in Figure 1 of main text. r_1 is the length of the aromatic bond on the benzene ring, r_2 is the length of the C−C bond between the triply coordinated atom and its doubly coordinated neighbor, r_3 is the length of the $C \equiv C$ triple bond, and r_4 is the length of the bond between adjacent carbon triple bonds. There are only two kinds of angles (120° and 180°) in the initial states for the three structures, but they all changed under strain. θ_1 is an internal angle of the benzene ring, and θ_2 is the angle on the alkyne-containing chain and links the aromatic bond with the triple bond. All the other angles can be deduced from θ_1, θ_2 or are nearly invariable, so they are ignored. When uniaxial strain is applied, the original D_{6h} $(P6/mmm)$ symmetry is transformed into rhombic D_{2h} $(Pmmm)$ symmetry. However, if shear strain is applied, the symmetry will reduce to monoclinic C_{2h} $(P2/m)$. To relax the strained structure, the bond lengths and angles changed differently between uniaxial strain and shear strain, leading to the different behaviors of the vibrational frequencies.

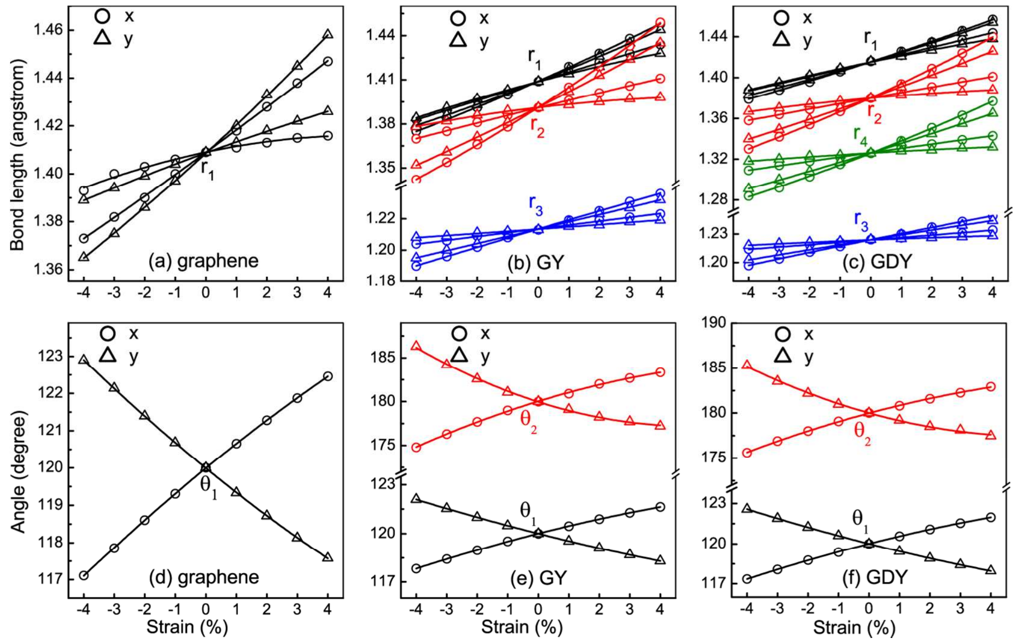

Figure S1. Variations in bond lengths and angles with uniaxial strain. The bond lengths of graphene, GY, and GDY are shown in (a), (b), and (c); the bond angles of those are shown in (d), (e), and (f). Squares and triangles correspond to the values under uniaxial strain in the x and y directions, respectively. Different colors correspond to different bond lengths or angles.

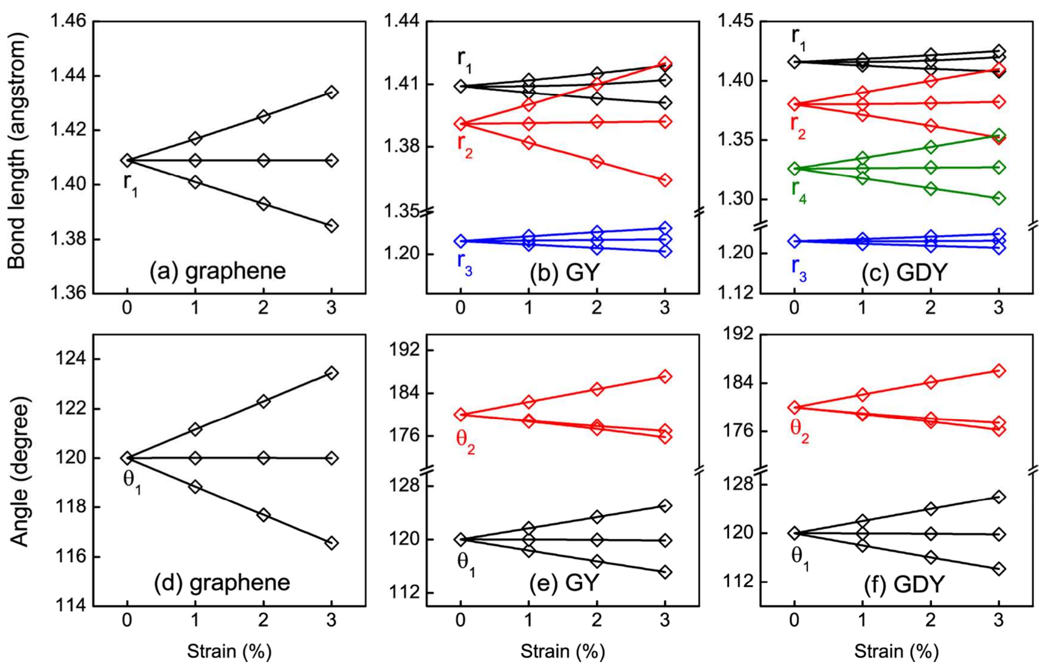

Figure S2. Variations in bond lengths and angles with shear strain. The bond lengths of graphene, GY, and GDY are shown in (a), (b), and (c); the bond angles are shown in (d), (e), and (f). Squares and triangles correspond to the values under uniaxial strain in x and y directions. Different colors correspond to different bond lengths or angles.

4) **The effects of van der Waals interactions on the frequency of G band.**

We adopte the non-local van der Waals density functional (vdW-DF) and explored the performance of vdW-DF combined with PBE functional to investigate the effects of vdW interactions. Table R1 shows the frequencies of G peaks for graphene, GY and GDY by different methods based on optimized structures.

Table S3. The frequency of G band by different methods (cm^{-1}).

	ω(graphene)	ω(GY)	ω(GDY)	ω(GY) −ω(graphene)	ω(GDY) −ω(graphene)
LDA	1620	1464	1520	-156	-100
PBE	1568	1418	1478	-150	-90
PBE+vdW	1557	1398	1457	-159	-100