6. Resultados

Siguiendo los pasos anteriormente mencionados (véanse para más detalle los cálculos con Mathematica recogidos en el anexo) se obtienen las siguientes matrices de constantes de fuerza:

$$\Phi^{01} = \begin{pmatrix} -\alpha 1 & 0 & 0 \\ 0 & -\frac{6\gamma 1}{d^2} & 0 \\ 0 & 0 & -\frac{3\gamma 2}{d^2} \end{pmatrix} \tag{27a}$$

$$\Phi^{02} = \begin{pmatrix} -\frac{\alpha 1}{4} - \frac{9\gamma 1}{2d^2} & \frac{\sqrt{3}\left(d^2\alpha 1 - 6\gamma 1\right)}{4d^2} & 0 \\ \frac{\sqrt{3}\left(d^2\alpha 1 - 6\gamma 1\right)}{4d^2} & \frac{3}{4}\left(-\alpha 1 - \frac{2\gamma 1}{d^2}\right) & 0 \\ 0 & 0 & -\frac{3\gamma 2}{d^2} \end{pmatrix} \tag{27b}$$

$$\Phi^{03} = \begin{pmatrix} -\frac{\alpha 1}{4} - \frac{9\gamma 1}{2d^2} & -\frac{\sqrt{3}\left(d^2\alpha 1 - 6\gamma 1\right)}{4d^2} & 0 \\ -\frac{\sqrt{3}\left(d^2\alpha 1 - 6\gamma 1\right)}{4d^2} & -\frac{3\alpha 1}{4} - \frac{3\gamma 1}{2d^2} & 0 \\ 0 & 0 & -\frac{3\gamma 2}{d^2} \end{pmatrix} \tag{27c}$$

$$\Phi^{04} = \begin{pmatrix} \frac{3\gamma 1}{4d^2} & -\frac{\sqrt{3}\gamma 1}{4d^2} & 0 \\ \frac{\sqrt{3}\gamma 1}{4d^2} & -\frac{4d^2\alpha 2 + \gamma 1}{4d^2} & 0 \\ 0 & 0 & -\frac{\delta}{3d^2} \end{pmatrix} \tag{27d}$$

$$\Phi^{05} = \begin{pmatrix} -\frac{3\alpha 2}{4} & \frac{\sqrt{3}\left(d^2\alpha 2 + 2\gamma 1\right)}{4d^2} & 0 \\ \frac{\sqrt{3}\alpha 2}{4} & \frac{1}{4}\left(-\alpha 2 + \frac{2\gamma 1}{d^2}\right) & 0 \\ 0 & 0 & -\frac{\delta}{3d^2} \end{pmatrix} \tag{27e}$$

$$\Phi^{06} = \begin{pmatrix} -\frac{3\alpha 2}{4} & -\frac{\sqrt{3}\left(d^2\alpha 2 + 2\gamma 1\right)}{4d^2} & 0 \\ -\frac{\sqrt{3}\alpha 2}{4} & \frac{1}{4}\left(-\alpha 2 + \frac{2\gamma 1}{d^2}\right) & 0 \\ 0 & 0 & -\frac{\delta}{3d^2} \end{pmatrix} \tag{27f}$$

$$\Phi^{07} = \begin{pmatrix} \frac{3\gamma 1}{4d^2} & \frac{\sqrt{3}\gamma 1}{4d^2} & 0 \\ -\frac{\sqrt{3}\gamma 1}{4d^2} & -\frac{4d^2\alpha 2 + \gamma 1}{4d^2} & 0 \\ 0 & 0 & -\frac{\delta}{3d^2} \end{pmatrix} \tag{27g}$$

$$\Phi^{08} = \begin{pmatrix} -\frac{3\alpha 2}{4} & \frac{\sqrt{3}\alpha 2}{4} & 0 \\ \frac{\sqrt{3}\left(d^2\alpha 2 + 2\gamma 1\right)}{4d^2} & \frac{1}{4}\left(-\alpha 2 + \frac{2\gamma 1}{d^2}\right) & 0 \\ 0 & 0 & -\frac{\delta}{3d^2} \end{pmatrix} \tag{27h}$$

$$\Phi^{09} = \begin{pmatrix} -\frac{3\alpha 2}{4} & -\frac{\sqrt{3}\alpha 2}{4} & 0 \\ -\frac{\sqrt{3}\left(d^2\alpha 2 + 2\gamma 1\right)}{4d^2} & \frac{1}{4}\left(-\alpha 2 + \frac{2\gamma 1}{d^2}\right) & 0 \\ 0 & 0 & -\frac{\delta}{3d^2} \end{pmatrix} \tag{27i}$$

Y dado que en el átomo 0 se tiene que cumplir el equilibrio,

$$\Phi^{00} = -\sum_{i=1}^{i=9} \Phi^{0i} = \begin{pmatrix} \frac{3}{2}\left(\alpha 1 + 2\alpha 2 + \frac{5\gamma 1}{d^2}\right) & 0 & 0 \\ 0 & \frac{3}{2}\left(\alpha 1 + 2\alpha 2 + \frac{5\gamma 1}{d^2}\right) & 0 \\ 0 & 0 & \frac{9\gamma 2 + 2\delta}{d^2} \end{pmatrix} \tag{28}$$

Los valores numéricos de las matrices, sustituidos los valores de las constantes proporcionados por los experimentos de Aizawa para el grafeno, pueden consultarse en el anexo.