Estado Sólido Avanzado
Tarea 02: Teoría de Bandas Electrónicas

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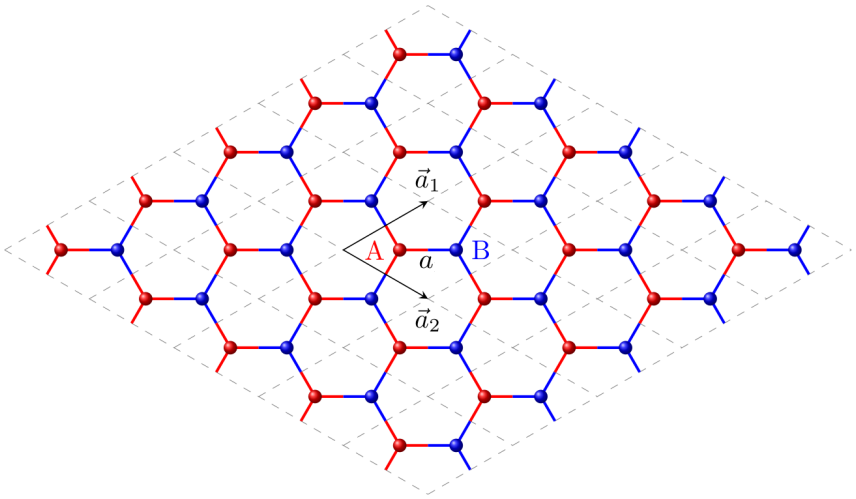
Problema 1 *Graphene: tight-binding approach*

Graphene is a $2D$ crystal with a $2-$atom basis located at $r_A = a\,(1,0)$ and $r_B = a\,(2,0)$, with $a = 1.42$ Å as the carbon-carbon distance, where its lattice vectors are given by,

$$\mathbf{a}_1 = \frac{a}{2}\left(3, \sqrt{3}\right), \qquad \mathbf{a}_2 = \frac{a}{2}\left(3, -\sqrt{3}\right).$$



Considering that each carbon contributes with four orbitals (s, p_x, p_y, p_z), calculate and plot the band structure for graphene, up to first-nearest neighbors, using the following overlap parameters (Popov *et al.*, Phys. Rev. B **70**, 115407 (2004)):

$$V_{ss\sigma} = -4.80 \text{ eV}, \qquad V_{sp\sigma} = 4.75 \text{ eV}, \qquad V_{pp\sigma} = 4.39 \text{ eV}, \qquad V_{pp\pi} = -2.56 \text{ eV}.$$

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