Estado Sólido I
Tarea 2: Enlace Químico

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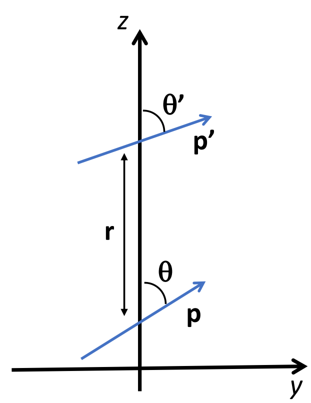
Problema 1 *van der Waals interaction by electric dipoles*

(a) An electric dipole, with dipolar moment $\mathbf{p}$, generates a potential energy $V(r)$ and electric field $\mathbf{E}$ given by:

$$V(r) = \frac{\mathbf{p}\cdot\mathbf{r}}{4\pi\epsilon_0 r^3}; \quad \mathbf{E} = -\nabla V(r).$$

Obtain the expresions for $V(r)$ and $\mathbf{E}$ in polar coordinates, if the electric dipole is oriented along the z-axis.

(b) The system is conformed by a couple of electric dipoles at fixed positions, separated by a distance $\mathbf{r}$, that are able to rotate on the plane zy, as depicted on the figure:



Calculate the potential energy $U_p = -\mathbf{p}'\cdot\mathbf{E}^p$ that feels the dipole $\mathbf{p}'$ under the influence of the electric field $\mathbf{E}^p$ generated by the dipole $\mathbf{p}$, as well as the torque $\boldsymbol{\tau}^{p'} = \mathbf{p}'\times\mathbf{E}^p$ exerted by $\mathbf{p}$ on $\mathbf{p}'$, and the torque $\boldsymbol{\tau}^{p} = \mathbf{p}\times\mathbf{E}^{p'}$ exerted by $\mathbf{p}'$ on $\mathbf{p}$.

(c) Find the stable equilibrium positions of the dipoles (angles θ and θ') as well as the minimum of potential energy U_p, assuming that the dipoles can rotate on the plane zy, but cannot translate.

(d) Consider that, in fact, the dipole $\mathbf{p}'$ is induced by the electric field $\mathbf{E}^p$ generated by the dipole $\mathbf{p}$: $\mathbf{p}' = \epsilon_0\alpha\mathbf{E}^p$, where α is the polarizability of the dipole $\mathbf{p}'$. Show that the potential energy of the two dipoles can be given by $U_p = -D/r^6$, and find D for the stable equilibrium positions at the minimum of potential energy.

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Problema 2 *Cohesive energy of bcc and fcc neon*

Using the Lennard-Jonnes potential, calculate the ratio of the cohesive energies of Neon (Ne) in the bcc and fcc structures. The lattice sums for the bcc are:

$$\Sigma'_j p_{ij}^{-12} = 9.11418; \quad \Sigma'_j p_{ij}^{-6} = 12.2533.$$

and for the fcc are:

$$\Sigma'_j p_{ij}^{-12} = 12.13188; \quad \Sigma'_j p_{ij}^{-6} = 14.45392.$$

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Problema 3 *Linear ionic crystal*

Consider a line of $2N$ ions of alternating charge $\pm q$ with a repulsive potential energy A/R^n only between first nearest neighbors.

(a) Show that at the equilibrium separation R_0:

$$U(R_0) = -\frac{2Nq^2 \ln 2}{R_0}\left(1 - \frac{1}{n}\right).$$

(b) Let the crystal be compressed so that $R_0 \to R_0(1-\delta)$ with $\delta \ll 1$. Show that the work done in compressing a unit length of the crystal has the leading term $C\delta^2/2$, where

$$C = \frac{(n-1)q^2 \ln 2}{R_0}.$$

Hint 01: The expressions are in CGS units. To obrain results in SI, replace q^2 by $q^2/4\pi\epsilon_0$.
Hint 02: Remember that $\ln(1+x) = \sum_{n=1}^{\infty}(-1)^{n+1}x^n/n$.

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Problema 4 *Equations of State*

For each of the following equations of state, calculate the $p(V)$ equation:

(a) EOS2:

$$E(V) = a + bV^{-1/3} + cV^{-2/3} + dV^{-1}.$$

(b) Murnagham EOS:

$$E(V) = E_0 + \frac{B_0 V}{B'}\left[\left(\frac{V_0}{V}\right)^{B'} \frac{1}{B'-1} + 1\right] - \frac{B_0 V_0}{B'-1}.$$

(c) Birch-Murnagham EOS:

$$E(V) = E_0 + \frac{9B_0V_0}{16}\left\{\left[\left(\frac{V_0}{V}\right)^{2/3} - 1\right]^3 B' + \left[\left(\frac{V_0}{V}\right)^{2/3} - 1\right]^2 \left[6 - 4\left(\frac{V_0}{V}\right)^{2/3}\right]\right\}.$$

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