Estado Sólido I
Tarea 1: Enlace Químico

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Problema 1 *Van der Waals interaction*

As a simple quantum mechanical model for the van der Waals interaction consider two identical harmonic oscillators (oscillating dipoles) at a separation R. Each dipole consists of a pair of opposite charges whose separations are x_1 and x_2, respectively, for the two dipoles. A restoring force f acts between each pair of charges ($f = -kx$).

(a) Write down the Hamiltonian H_0 for the two oscillators without taking into account electrostatic interaction between the charges.

(b) Determine the interaction energy H_1 of the four charges.

(c) Assuming $|x_1| \ll R$ and $|x_2| \ll R$, approximate H_1 as follows

$$H_1 \approx -\frac{2e^2 x_1 x_2}{R^3},$$

(d) Show that tranformation to normal coordinates, $x_s = (x_1 + x_2)/\sqrt{2}$ and $x_a = (x_1 - x_2)/\sqrt{2}$, decouples the total energy $H = H_0 + H_1$ into a symmetric and an antisymmetric contribution.

(e) Calculate the frequencies ω_s and ω_a of the symmetric and antisymmetric normal vibration modes. Evaluate the frequencies ω_s and ω_a as Taylor series in $2e^2/(kR^3)$ and truncate the expansions after second order terms.

(f) The energy of the complete system of two interacting oscillators can be expressed as $U = \hbar(\omega_s + \omega_a)/2$. Derive an expression for the energy of the isolated ocillators and show that this is decreased by an amount c/R^6 when mutual interaction (bonding) occurs.

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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 between nearest neighbors.

(a) Show that at the equilibrium separation

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

(b) Let the crystal be compressed so that $R_0 \to R_0(1-\delta)$. 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: the expressions are in CGS units. To obrain results in SI, replace q^2 by $q^2/4\pi\epsilon_0$.

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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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