Estado Sólido I
Tarea 2: Enlace Químico

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Nombre del Estudiante: ______________________________

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 ($f = -Cx$).

(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 transformation 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 $2e^2/(CR^3)$ 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 oscillators and show that this is decreased by an amount cte$/R^6$ when mutual interaction (bonding) occurs.

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Problema 2 *Lattice sums for the cubic structure*

For a cubic structure, the lattice sums' exact values for the Lennard-Jones potential are the following:

$$\Sigma_j' p_{ij}^{-12} = 6.2021; \quad \Sigma_j' p_{ij}^{-6} = 8.4019.$$

(a) Calculate both lattice sums (12- and 6-power) for different number of neighbors (first, second, and so on), and find the one with a difference of less than 0.02% for the 12-power sum, respect to the exact value.

(b) How much is the difference for the 6-power sum of the number of neighbors determined on the previous question (respect to the exact value)?

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Problema 3 *Bonding properties for an ionic crystal*

The repulsive interaction for an ionic crystal can be also be expressed by the model of Born-Meyer, giving for the total energy of the crystal the following:

$$U(R) = N\left[\beta\left(\frac{R_0}{R}\right)^n - \frac{\alpha q^2}{R}\right],$$

where N is the number of ion pairs in the crystal, R_0 is the equilibrium first nearest-neigborns distance, and α and β are material-related parameters.

(a) Obtain a relationship between the α and β parameters, considering that the system is in equilibrium.

(b) Determine an expresion for the bulk modulus (B_0) in the equilibrium.

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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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