Estado Sólido I
Tarea 2: Enlace Químico

Dr. Omar De la Peña Seaman

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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. In particular for the NaCl crystal (B1 structure),:

(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 *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 W in compressing a unit length of the crystal has the leading term $C\delta^2/2$, where

$$C = \frac{(n-1)q^2 \ln 2}{R_0} \quad \forall \quad W = U[R_0(1-\delta)] - U(R_0).$$

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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