HW1

Kovalev Vyacheslav

(1). The ionization energy of lithium is 5.4 eV and the electron affinity of iodine is -295 $kJ \cdot mol^{-1}$. Calculate the cohesive energy of LiI diatomic molecule, if equilibrium separation distance between ions is 0.238 nm.

$$295\ kJ \cdot mol^{-1} = 295 * \frac{10^3}{1.6 * 10^{-19} * \ 6 * 10^{23}} = 3\frac{eV}{particle}$$

$$\begin{cases} Li + 5.4eV \rightarrow Li^+ + e^- \\ I + e^- \rightarrow I^- + 3eV \end{cases} =>$$

$$Li + I + 5.4eV \rightarrow Li^+ + I^- + 3eV =>$$

$$Li + I + 2.4eV \rightarrow Li^+ + I^- =>$$

$$U_{min} = -k\frac{e^2}{r_0} = -9 * 10^9 \frac{[1.6 * 10^{-19}]^2}{0.238nm} = -9.6 * 10^{-19}J = -6eV$$

The cohesive energy = 2.4 – 6 = - 3.6 eV

(2). Calculate the total surface area of graphene flakes with a total mass of m = 1 g, if it is known that the distance between the nearest carbon atoms is a = 0.142 nm, and the carbon atomic mass is mC = 1.994·10-26 kg.

Surface of regular hexagon is $S = \frac{3\sqrt{3}}{2}a^2 = 0.52nm^2 = 5.2 * 10^{-20}$

For each cell we have 6 atoms each is shared between 3 cells therefore total concentration of atoms is $\rho = \frac{6}{3} = 2$

count of cells is $N = \frac{m}{mC*\rho} = 2.5 * 10^{22}$

$$S_{total} = S * N = 1313м^2$$

I calculated S on one side.

(3). Derive the expression and calculate the numerical value of the constant indicated in Wien's law:

$$Umax \ = \ constant \cdot T^5$$

$I_\nu = \frac{2h\nu^3n^2}{c_0^2}\frac{1}{\exp\left(\frac{h\nu}{kT}\right)-1}$ –Planck's formula

$$\nu = \frac{c_0}{n\lambda}\ and\ U_\nu|d\nu| = U_\lambda|d\lambda| =>$$

$$I_\lambda = \frac{c_0}{n\lambda^2}I_\nu = \frac{c_0}{n\lambda^2}\frac{2h\nu^3n^2}{c_0^2}\frac{1}{\exp\left(\frac{h\nu}{kT}\right) - 1} = \frac{2hc_0^2}{n^2\lambda^5}\frac{1}{\exp\left(\frac{hc_0}{nk\lambda T}\right) - 1}$$

$$C_1 = 2hc_0^2, \qquad C_2 = \frac{hc_0}{k}$$

$$I_\lambda = \frac{C_1}{n^2\lambda^5}\frac{1}{\exp\left(\frac{C_2}{n\lambda T}\right) - 1}$$

I_λ represents the amount of radiation energy emitted by the black body surface at temperature T per unit time.

The Wien displacement law: at wavelength λ_{max} to which corresponds the max of surface density of an emitted energy flux.

From Planck function:

$$\lambda_{max}T = \frac{C_2}{5}\frac{1}{1 - \exp\left(-\frac{C_2}{\lambda_{max}T}\right)}$$

Solution: $\lambda_{max}T = C_3$

Substitute in I_λ

$$I_{\lambda_{max}} = T^5\frac{C_1}{n^2(\lambda_{max}T)^5}\frac{1}{\exp\left(\frac{C_2}{n\lambda_{max}T}\right) - 1} = T^5\frac{C_1}{n^2C_3^5}\frac{1}{\exp\left(\frac{C_2}{nC_3}\right) - 1} =$$

$$= T^5 * const$$

(4). For a particle in a cubic three-dimensional potential box, calculate the degree of degeneracy of the 7th energy level.

Suppose $\psi = X(x)Y(y)Z(z)$

$$\nabla^2\psi + \frac{2m}{\hbar}E\psi = 0$$

$$\frac{1}{\psi}\nabla^2\psi + \frac{2m}{\hbar}E = 0$$

Divide into parts with corresponding dependencies of x,y,z and substitute $K^2 = \frac{2m}{\hbar}E$

$$\frac{1}{X}\frac{d^2X}{dx^2} = -K_x^2$$

$$X = A_x cos(K_x x) + B_x \sin(K_x x)$$

$$X(0) = 0 => A_x = 0$$

$$X(a) = 0 => K_x a = n_x \pi => K_x = \frac{n_x\pi}{a}$$

$$X = B_x \sin\left(\frac{n_x\pi x}{a}\right)$$

The same for Y,Z =>

$$\psi = B\sin\left(\frac{n_x\pi x}{a}\right)\sin\left(\frac{n_y\pi y}{a}\right)\sin\left(\frac{n_z\pi z}{a}\right)$$

$$E = \frac{\hbar^2}{2m}\left(K_x^2 + K_y^2 + K_z^2\right) = \frac{h^2}{8ma^2}\left(n_x^2 + n_y^2 + n_z^2\right)$$

$$n^2 = n_x^2 + n_y^2 + n_z^2$$

energy levels:

1. (1,1,1) n^2 = 3
2. (1,1,2), (1,2,1), (2,1,1) n^2= 6
3. (1,2,2), … n^2 = 9
4. (1,1,3), …   n^2=11
5. (2,2,2)   n^2=12
6. (3,2,1) …   n^2 =14
7. (2,2,3), (3,2,2), (2,3,2)   n^2=4+4+9 =17

$$E_7 = \frac{h^2}{8ma^2}(n^2) = \frac{17h^2}{8ma^2}$$

degree of degeneracy = 3

(5). An electron is bound in a cubic three-dimensional infinite potential well of side 1×10-10m. Find the energy values in the ground state and first two excited states.

$$m_e = 9.1093837 \times 10^{-31}$$

From prev task take formula and states:

$$E = \frac{h^2 n^2}{8m_e a^2}$$

$$h = 6{,}626\ 070\ 15 \times 10^{-34}\ J/s$$

$$a = 1 * 10^{-10} m$$

$$E_1 = \frac{h^2 3}{8m_e a^2} = 1.8 * 10^{-17} J = 112\ eV$$

$$E_2 = \frac{h^2 6}{8m_e a^2} = 224 eV$$

$$E_3 = \frac{h^2 9}{8m_e a^2} = 336 eV$$

(6). Calculate the velocity and kinetic energy of an electron of de-Broglie wavelength 1.66×10-10m

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2Em}} => \sqrt{2Em} = \frac{h}{\lambda} => E = \frac{h^2}{2m\lambda^2}$$

All values in prev task:

$$E = \frac{h^2}{2m\lambda^2} = 8.7\ * 10^{-18} J = \ 54 eV$$

$$E = \frac{1}{2} m v^2 =>$$

$$v = \sqrt{\frac{2E}{m}} = 4369124 \frac{m}{s}$$