Organic Electronic Devices

Week 2: Electronic Structure
Tutorial 2.1: Homework Solutions

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Solutions to Problem 1

• Problem Statement

The energy associated with vacuum (i.e., the absence of matter) is defined to be 0 eV in many organic electronic systems and all energies are referenced as negative values removed from that 0 eV level. The HOMO level of a newly-synthesized π-conjugated polymer resides at –5.2 eV. Researchers have illuminated a thin film of this polymer with a number of different wavelengths of light, and they have found that the longest wavelength of light that will excite an electron from the HOMO level of the polymer to the LUMO level of the polymer is 800 nm. Determine the band gap and the absolute position of the LUMO level, which is defined to be closer to 0 (i.e., less negative) than the HOMO level, of the new polymer if photon energy (E) is related to wavelength by the following equation.

\[ E = \frac{hc}{\lambda} \]

Where \( h \) is Planck’s constant, \( c \) is the speed of light, and \( \lambda \) is the wavelength of the incident photon.
Band Gap Energy

\[ E = \frac{hc}{\lambda} = \left(4.135 \times 10^{-15} \text{ eV s}\right) \times \left(2.998 \times 10^{17} \text{ nm}\right) \div 800 \text{ nm} \]

\[ E = 1.55 \text{ eV} \]

Band Gap Energy \((E_g) = 1.55 \text{ eV}\)

HOMO Energy = –5.2 eV

LUMO Energy = –3.65 eV
Solutions to Problem 2

• Problem Statement

The energy \((E)\) associated with a particle in a specific quantum state \((n)\) of a 1-dimensional box is given by the following equation.

Here, \(h\) is Planck’s constant \((6.626 \times 10^{-34} \text{ m}^2 \text{ kg}^{-1} \text{ s}^{-1})\), \(m\) is the mass of the particle, and \(L\) is the length of the box. Calculate the energy required for a particle to increase from the third to the fourth quantum state in this simple model if the mass of the particle is \(9.109 \times 10^{-31} \text{ kg}\) and the length of the box is \(1.0 \text{ nm}\).

\[
E_n = \frac{n^2 h^2}{8 mL^2}
\]

• Solution

\[
\Delta E_n = \left(\frac{n_4^2 - n_3^2}{8 mL^2}\right)h^2 = \left(\frac{16 - 9}{8 mL^2}\right)h^2
\]
Solutions to Problem 2 (Continued)

- Solution

\[ \Delta E_n = \frac{(n_4^2 - n_3^2)h^2}{8mL^2} = \frac{(16 - 9)h^2}{8mL^2} \]

\[ \Delta E_n = \frac{7 \left( 6.626 \times 10^{-34} \ m^2 \ kg \ s^{-1} \right)^2}{8 \left( 9.109 \times 10^{-31} \ kg \right) \left( 1 \times 10^{-9} \ m \right)^2} \]

\[ \Delta E_n = 4.22 \times 10^{-19} \ m^2 \ kg \ s^{-2} = 4.22 \times 10^{-19} \ J \]

\[ \Delta E_n = 2.63 \ eV \]
Solutions to Problem 3

• Problem Statement

Using the simple model shown in the course for 1,3-butadiene, show that the length of 1,3,5-hexatriene can be estimated to be 0.867 nm. Estimate the amount of energy in the first electronic transition (in eV) for 1,3,5-hexatriene.

• Solution

1,3,5-Hexatriene
6 Carbons with sp² Hybridized Orbitals

\[ \Delta E_n = \frac{\left( n_{\text{final}}^2 - n_{\text{initial}}^2 \right) \hbar^2}{8 m L^2} \]

Assume that the Molecule is Linear (i.e., Do Not Consider Bond Angles)

3 C=C Double Bonds (0.135 nm): 0.405 nm
2 C-C Single Bond (0.154 nm): 0.308 nm
2 Carbon Radii (0.077nm): 0.154 nm

Summing These Values Gives \( L \)

\[ L = 0.867 \text{ nm} \]
1,3,5-Hexatriene
6 Carbons with sp² Hybridized Orbitals

Assume that the Molecule is Linear (i.e., Do Not Consider Bond Angles)

3 C=C Double Bonds (0.135 nm): 0.405 nm
2 C-C Single Bond (0.154 nm): 0.308 nm
2 Carbon Radii (0.077 nm): 0.154 nm

Summing These Values Gives $L$

$L = 0.867 \text{ nm}$

\[
\Delta E_n = \frac{\left(n_{\text{final}}^2 - n_{\text{initial}}^2\right)\hbar^2}{8mL^2}
\]

\[
\Delta E_n = \frac{(16 - 9)\hbar^2}{8mL^2}
\]

$\Delta E_n = 3.50 \text{ eV}$
Solutions to Problem 4

• Problem Statement

  • For an intrinsic sample of Ge at T = 298 K, calculate the carrier concentration if: \( E_g = 0.66 \text{ eV} \), \( N_c = 1.05 \times 10^{25} \text{ m}^{-3} \), and \( N_v = 3.92 \times 10^{24} \text{ m}^{-3} \). Assume room temperature conditions.

• Solution

\[
n_i^2 = N_c N_v \times \exp \left[ \frac{(-E_g)}{kT} \right]
\]

\[
n_i^2 = \left(1.05 \times 10^{25} \text{ m}^{-3}\right) \times \left(3.92 \times 10^{24} \text{ m}^{-3}\right) \times \exp \left[ \frac{(-0.66 \text{ eV})}{(0.026 \text{ eV})} \right]
\]

\[
n_i^2 = 3.98 \times 10^{38} \text{ m}^{-6}
\]

\[
n_i = 1.97 \times 10^{19} \text{ m}^{-3}
\]