Polymer Science — Physical & Engineering Properties
Submission on July 12th and discussion on July 13th, 2022 — Problem Set 4
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Topic: π Conjugated Polymers and Charge Transport

1) The π electrons along a conjugated segment of a polymer can be considered as a one-dimensional system of length ℓ, with ℓ being the total length of the segment.
   a) How many π type molecular orbitals does one get for a system comprising 2N sp2 hybridized carbon atoms? How many of these orbitals are occupied by electrons?
   b) The energy of the nth molecular orbital of a π conjugated system can be estimated by the "particle in a box" model (infinite potential well model). Here, the energy of the nth level is given by
   $$E_n = \frac{h^2 n^2}{8 m_e \ell^2}.$$
   Please show that the energy gap is defined as
   $$\Delta E = \frac{h^2}{16 m_e N L^2}$$
   where 2N is the number of carbon atoms and $L = 1.39$ Å is the average length of a C–C bond in the conjugated segment. (You may want to use the approximation $N \gg 1$ or $\frac{1}{N} \gg \frac{1}{N^2}$.)
   c) What number of carbon atoms is needed to give the lowest absorption wavelength at 510 nm according to that model?

2) Solid PMMA has a refractive index $n_{PMMA} = 1.49$ at a wavelength of 632 nm. Its mass density is $\varrho = 1.19\ \frac{\mathrm{g}}{\mathrm{cm}^3}$ and each repeat unit has a molar mass of $100\ \frac{\mathrm{g}}{\mathrm{mol}}$.
   a) Calculate the polarizability per repeat unit.
   b) How large is the electric dipole moment induced by an electric field $E = 10^8\ \frac{\mathrm{V}}{\mathrm{m}}$?
   c) How does the polarizability volume compare with the real volume of the monomer unit?