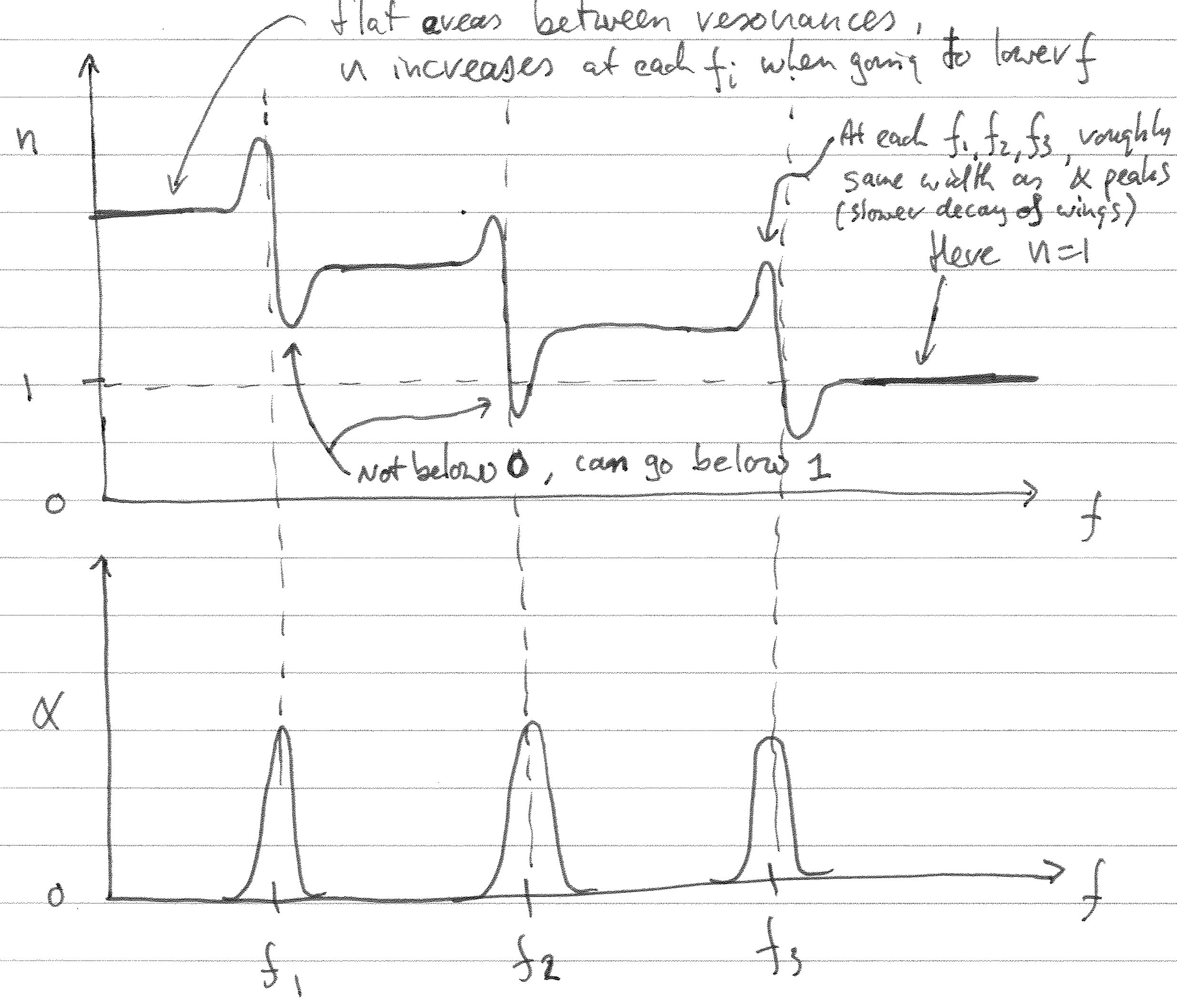
Model Answers Exam
Functional Properties – Optical Materials
26 Jan 2018

Problem 1-opt

a)



b) The resonances f_2 and f_3 are at visible and UV frequencies. These typically correspond to electronic transitions. The resonance at f_1 is at infrared frequency, and could thus very well be a vibronic transition (lattice phonons).

c) It is not a metal or semiconductor, since there is never a wide band with strong absorption.
It is probably not a molecular material, since these mostly have broader resonances and also broad phonon (vibronic) side bands (or phonon replicas) for f_2 and f_3.
It could very well be a glass or crystalline insulator. Then f_1 is a distinct vibronic mode, and f_2, f_3 correspond to electronic transitions of localized impurity states.
f_3 is not an electronic transition of bulk material, since there is no increasing absorption for $f > f_3$.
Apperently, this material is mostly transparent for $f > f_3$. That must be a material with a very large bandgap (indirect), and little X-ray absorption (light nuclei).

d) Estimate n for $f_n = 3 \times 10^{15}$ Hz $\Rightarrow$ is between f_2 and f_3.
$\Rightarrow$ Only increas of n above 1 due to the resonance at f_3.
Well below f_3, we can use the approximation

$$\Delta \varepsilon = \varepsilon(f_n) - \varepsilon(\infty) = \varepsilon(f_n) - 1 = \frac{N_3 e^2}{\varepsilon_0 m_0 \omega_0^2}$$

Use here $\omega_0 = 2\pi f_3$
m_0 is electron mass

$\Rightarrow$

$$n \approx \sqrt{\varepsilon(f_n)} = \sqrt{1 + \Delta\varepsilon}$$

$$= \sqrt{1 + \frac{N_3 e^2}{\varepsilon_0 m_0 (2\pi f_3)^2}} \underset{\text{numbers}}{\overset{\text{fill in}}{=}} 1.049$$

Problem 2-opt

a) The value of R_x is the energy difference between the $n=1$ free exciton absorption line $\left[\left(E_{gap} - \frac{R_x}{n^2}\right) \text{ for } n=1\right]$ and E_{gap} $\left[\text{that is, } \left(E_{gap} - \frac{R_x}{n^2}\right) \text{ for } n \to \infty\right]$.

$E_{gap} = E_g = 1.5192$ (read from plot)

$E_{X_{n=1}} = 1.5149$ (" " ")

$$R_x \approx 4.3 \text{ meV}$$

b) The Bohr radius of the free exciton is

$$r_n = \frac{m_0}{\mu} \varepsilon_r n^2 a_H ,$$

where a_H the Bohr radius of the Hydrogen atom for $n=1$, $a_H = 0.0529$ nm.

Here μ is the reduced mass for the electron-hole system,

$$\mu = \frac{1}{1/m_e^* + 1/m_h^*}$$

← Electron and hole effective mass

Filling in all numbers for r_n with $n=1$,

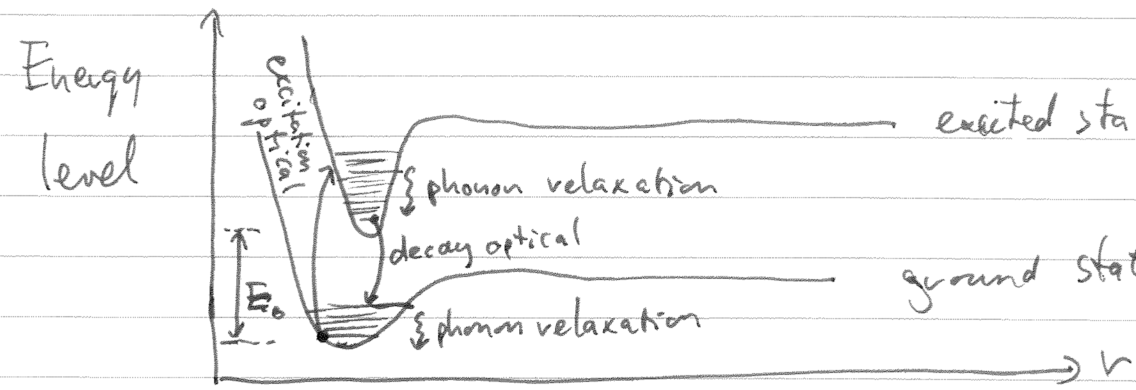
$m_e^* = 0.067\, m_0$, $m_h^* \approx 0.2\, m_0$, $\varepsilon_r = 12.8$

↑ estimate (any value $m_e^* \leq m_h^* \leq m_0$ is graded as correct)

gives $r_n = 13.5$ nm

Problem 3-opt

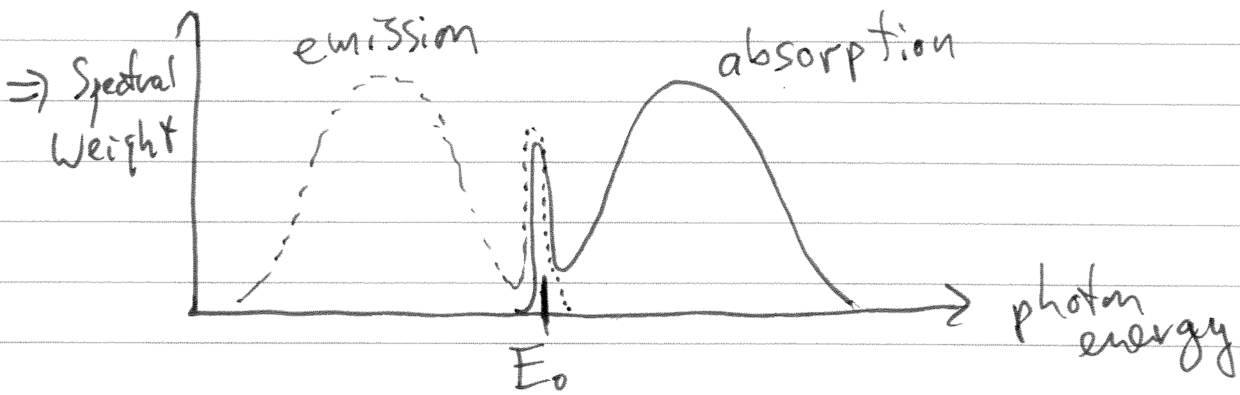
Molecules have strong electronic and vibronic resonances that are coupled. This can be represented in the following diagram



Separation between atoms in the molecule, for some relevant coordinate r

For optical excitation, there is strong absorption for photon energies $> E_0$, due to a process that generates both the electronic transition and phonons

For optical emission, a big part of the photons come out at energies $< E_0$, since it can decay to the electronic ground state to a level with high phonon excitation.



Problem 4-opt

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a)

Potential	Curve	Explanation
B	2	This is the most parabolic curve, so the most linear respons for the $P-\mathcal{E}$ relation
A	1	For this potential, the charged particles feel less restoring force at large displacement $\Rightarrow$ P increases super-linear at high $\mathcal{E}$ driving amplitudes
C	3	For this potential, the charged particles feel an enhanced restoring force at large displacement $\Rightarrow$ P increases sub-linear at high $\mathcal{E}$ driving amplitudes

b) $$\chi^{\text{non linear}} = \chi^{(1)} + \chi^{(2)}\mathcal{E} + \chi^{(3)}\mathcal{E}^2$$

$$P = \varepsilon_0\chi^{(1)}\mathcal{E} + \varepsilon_0\chi^{(2)}\mathcal{E}^2 + \varepsilon_0\chi^{(3)}\mathcal{E}^3 + \ldots\ldots$$

For each curve, the slope at $\mathcal{E} \approx 0$ is about the same and positive $\Rightarrow \chi^{(1)} > 0$ for all curves

For each curve, it is anti-symmetric about $\mathcal{E} = 0 \Rightarrow$ $\chi^{(2)} = 0$ for all three curves

For curve 2, $\chi^{(3)} = 0$ since it is linear.
For curve 1, $\chi^{(3)} > 0$, since it is super-linear.
For curve 3, $\chi^{(3)} < 0$, since it is sub-linear.

c) If P oscillates at ~~frequencies~~ $\neq \omega$,

this will cause the emission of EM fields at these different frequencies. For the case here, the response is dominated by $\chi^{(1)}$ and $\chi^{(3)}$.

Assume the driving field is $\mathcal{E} = \mathcal{E}_A \cos(\omega t)$ $\Rightarrow$

↑ amplitude.

$$P = \varepsilon_0 \mathcal{E}_A \chi^{(1)} \cos(\omega t) + \varepsilon_0 \mathcal{E}_A^3 \left(\cos(\omega t)\right)^3$$

$$\boxed{\text{Use} \quad \cos^3(x) = \tfrac{3}{4}\cos(x) + \tfrac{1}{4}\cos(3x)} \Rightarrow$$

$$P = \varepsilon_0 \mathcal{E}_A \chi^{(1)} \cos(\omega t) + \tfrac{3}{4}\varepsilon_0 \mathcal{E}_A^3 \chi^{(3)} \cos(\omega t) + \tfrac{1}{4}\varepsilon_0 \mathcal{E}_A^3 \cos(3\omega t)$$

P also oscillates at frequencies 3ω. The dominant frequencies in the response are ω and 3ω.