Problem Sheet 2 - Perovskites and Nanomaterials

Submission deadline: 1pm on 10th March 2025

Fundamental constants and formulae can be found in the Exam Summary Sheet (available on Moodle).

Problem 1

A 2D perovskite is formed with alternating layers of inorganic lead iodide octahedra and organic spacer cations. The thickness of each inorganic layer is 0.6 nm, and the thickness of each organic layer is 1.2 nm.

a) Calculate the effective band gap of the 2D perovskite, assuming that the band gap of the bulk lead iodide perovskite is 1.5 eV and that quantum confinement effects lead to a band gap increase inversely proportional to the square of the inorganic layer thickness. [3]

b) Discuss the advantages and disadvantages of using 2D perovskites in solar cells compared to 3D perovskites. [4]

Problem 2

a) Explain what is ion intermixing, giving advantages of this method over the conventional perovskite structure. [2]

b) Analyse the composition of the perovskite given by the formula:

$$(FA_{0.83}MA_{0.17})_{0.95}Cs_{0.05}Pb(I_{0.83}Br_{0.17})_3$$

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i) List all the components, clearly labelling their function in the perovskite structure (A, B, X, etc.) [3]

ii) For each component, give a rationale for using it in the material. [3]

iii) Estimate qualitatively the difference between the original material and:

i. $(FA_{0.83}MA_{0.17})_{0.95}Cs_{0.05}PbI_3$ [1]

ii. $MA_{0.95}Cs_{0.05}Pb(I_{0.83}Br_{0.17})_3$ [1]

iii. $FA_{0.83}MA_{0.17}Pb(I_{0.83}Br_{0.17})_3$ [1]

iv) Calculate the correct values of x, y and z in the perovskite formulae below.

i. $La(Al_xMg_{0.5}Ta_{0.25})O_3$ [1]

ii. $(La_xSr_{0.2})_y(Mn_{0.2}Fe_zCo_{0.4}Al_{0.2})O_3$ [3]

Problem 3

a) Compare and contrast charge carrier properties of hybrid perovskites and organic semiconductors. In particular, outline the difference in:

   (a) nature of charge carriers and their main properties [2]

   (b) importance of polarons for optoelectronic applications in both materials [2]

Problem 4

a) Briefly explain the importance of surface plasmon polaritons in nanomaterials applications. [2]

b) A silver nanostructure embedded in air ($\epsilon_{air} = 1$) is illuminated by a He-Ne laser ($\lambda_0 = 632.8$ nm). At this wavelength, silver has permittivity $\epsilon_m = -15.88$. Calculate the effective wavelength of surface plasmon polaritons in this nanostructure. [2]

c) A nanometer-sized optical cavity is formed by creating a thin layer of SiO_2 sandwiched between Au claddings. A red light ($\lambda = 651$ nm in vacuum) is confined in the cavity as a surface plasmon polariton with a wavelength of $\lambda_{eff} = 51$ nm.

   i calculate the effective refractive index of the cavity. [2]

   ii comment on viability of obtaining such refractive index in bulk materials. [1]

   iii Suggest two ways the cavity in the previous question could be applied outside of the lab. [2]