NanoElec exam – January 28th, 2021

Duration: 3 hours.

1 point per question (total = 37 pts)

Answer on Part A and Part B on two separate sheets.

Documents of the NanoElec course are allowed in pdf or in print: course, exercises

Part A – Molecular electronics & plasmonics

I. Fundamental understanding

Use the figure given in Appendix 1, where the Band diagram of GaAs is drawn.

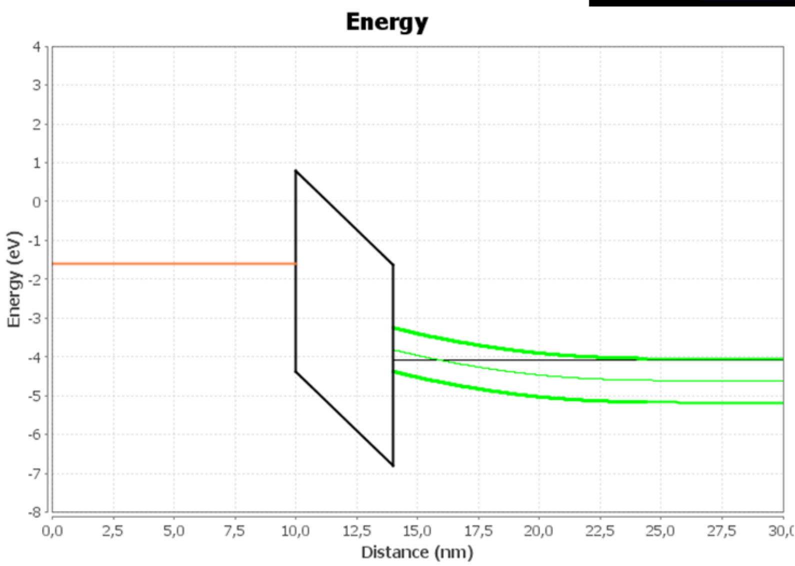
1. Draw on the diagram the process that occurs when a photon of energy $h\nu$ is absorbed by the GaAs crystal (you will need to hand over Fig. 1). Explain what happens.
2. Measure the value of the band gap.
3. Is GaAs a direct or an indirect semiconductor?
4. On this diagram, indicate where is the dispersion band of the light hole and that of the heavy holes?

5. Give the Ohm's law in its local form (link between density of current and local electric field).
6. Explain the difference between diffusive transport and ballistic transport
7. What is the Landauer formula? (equation and its significance)

II. MIS structure

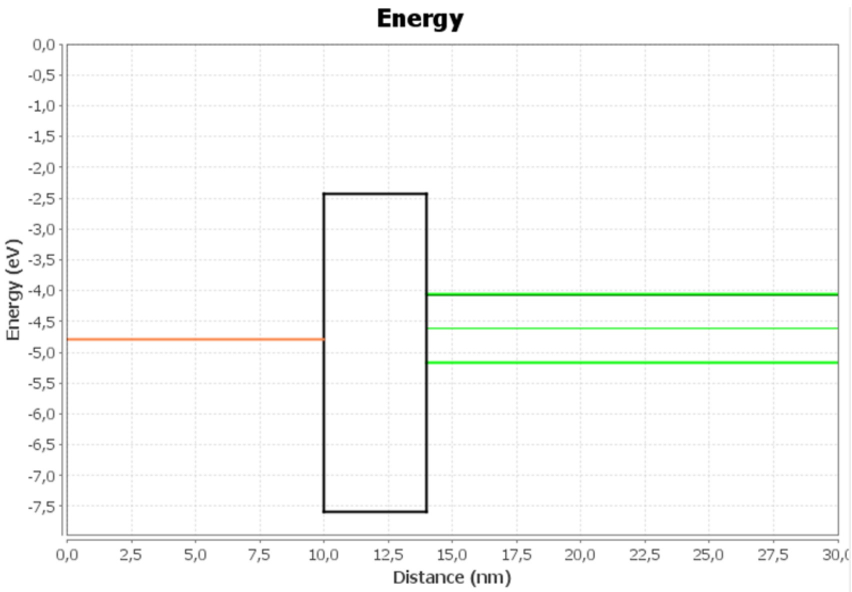
Consider an MIS structure made of a gold electrode, a thin layer of an organic molecule (nitrophenyl molecule) and a n-doped silicon. The silicon substrate is doped with phosphorus, with a donor density of 1E19 cm^{-3}. The silicon electrode is grounded.

1. The band diagram of this structure is calculated analytically and shown below, when a bias V_1 is applied to the gold electrode.
   Make a simple sketch of this junction, and indicate the bias voltage and the ground. What it the thickness of the organic layer?
2. From the graph below, what is the value of V_1?
3. Knowing that the work function of gold is 4.8 eV, draw the vacuum level. Indicate where there is an electric field. Where is this field the strongest?
4. What is the width W of the depletion layer (also called space charge region (give the value of W)?
5. Comment on the band bending regime of this MIS junction at this potential V_1 (depletion, inversion, etc.. and majority carrier at the interface)



The bias is changed to a new value V_{fb} and a new band diagram is calculated below.

6. What is special with the value of V_{fb} and what is its name? Estimate V_{fb}.
7. Use this graph below to give an estimate of the HOMO and LUMO of nitrophenyl.



III. Difurylethene-based photochromic single-molecule junctions

The following situations are taken from an article entitled “Inelastic electron tunneling spectroscopy of difurylethene-based photochromic single-molecule junctions”, authored by Youngsang Kim, Safa G. Bahoosh, Dmytro Sysoiev , Thomas Huhn , Fabian Pauly and Elke Scheer in 2017. (Beilstein J. Nanotechnol. 2017, 8, 2606–2614)

Diarylethene-derived molecules alter their electronic structure upon transformation between the *open* and *closed* forms of the diarylethene core, when exposed to ultraviolet (UV) or visible light. This transformation results in a significant variation of electrical conductance and vibrational properties of corresponding molecular junctions.

1. Explain the principle of the switching of this molecule with light.
2. The MCBJ is depicted in Fig 1-(a). Explain how the distance between the two electrode is controlled (draw some sketches if needed).
3. How is it possible to measure the conductance of a single molecule?
4. Explain how figure 1(d) is obtained. What are the values of the conductance of the open and closed states?
5. What would be the value of a single quantum point contact (QPC)? And why the values obtained here are much lower?

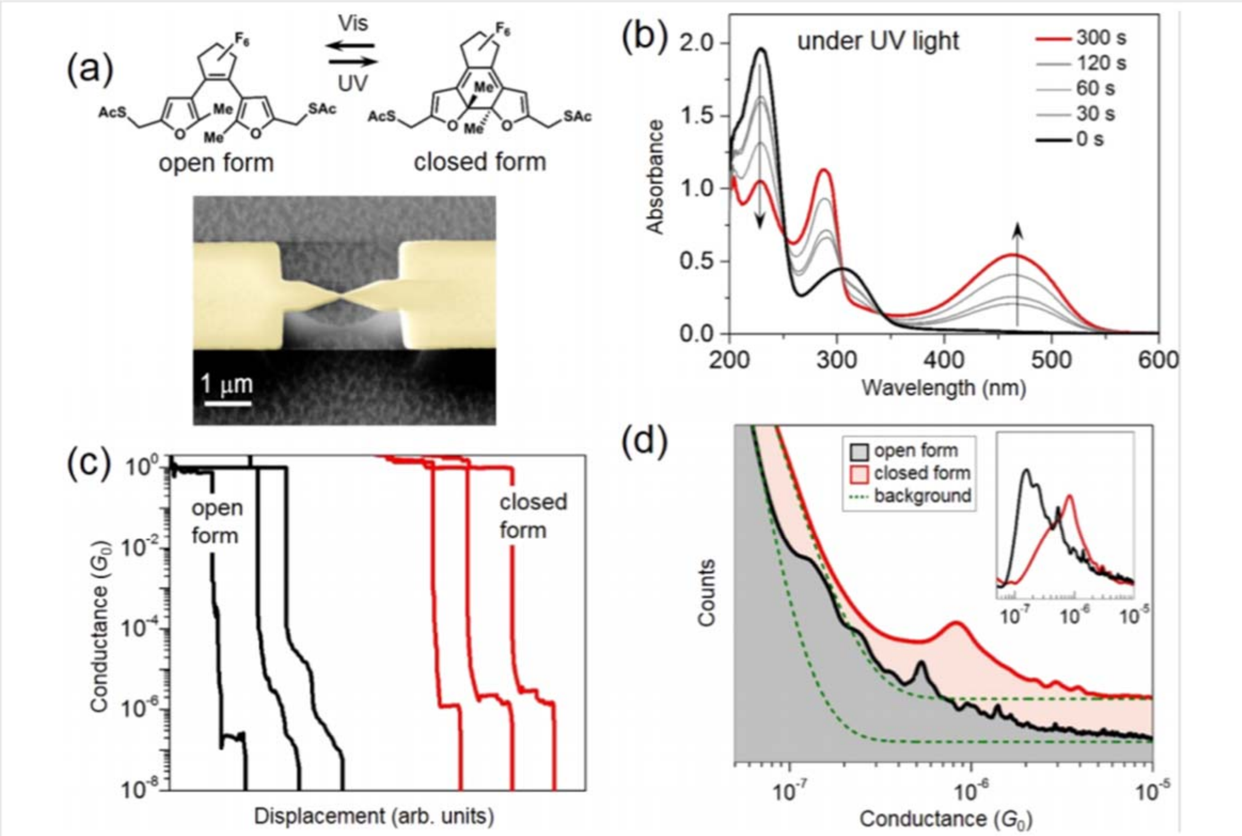
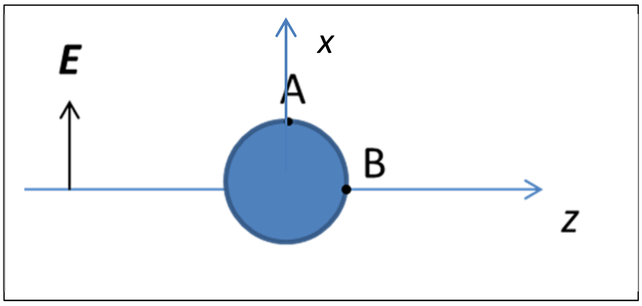


Figure 1: (a) Structures of the open and closed forms of difurylethene-thio-methyl (C5F-ThM) molecules, which switch states under the illumination with UV and visible light. Shown at the bottom is a scanning electron microscopy image of a MCBJ device. (b) Variation of UV–visible absorption spectra under UV light irradiation (wavelength of 313 nm with an intensity of ca. 0.15 mW/cm^{-2}) as a function of illumination time. The black curve corresponds to the open form, the red one to the closed form. (c) Conductance traces recorded while breaking C5F-ThM molecular junctions, containing the open form (black) and the closed form (red). Curves are shifted along the displacement axis for clarity. (d) Conductance histograms constructed from around 1000 curves of breaking and forming processes. The lowest conductances for the open and closed forms are $(1.4 \pm 1.0) \times 10^{-7}$ G_0 and $(8.3 \pm 4.5) \times 10^{-7}$ G_0, respectively. Histogram curves of both forms (black and red lines) are displaced along the counts axis for better visibility. The inset shows the corresponding conductance histograms after subtracting the exponential backgrounds indicated by green dashed lines in the main panel.

IV. Plasmonics. Amplification of the local field in the vicinity of a spherical nanoparticle.

Let's consider a light wave of wavelength λ_0 in vacuum, and a field amplitude $E_0\boldsymbol{u}_x$. We consider a spherical gold nanoparticle of radius *R*, much smaller than λ_0 so as to be in the quasi-static approximation. The particle is in vacuum.



Cylindrical coordinates are used, oriented along the $\boldsymbol{u}_x$ direction. Bleow is the expression of the electric field radiated by this particle at a distance *r* from the center of the particle (dipolar approximation):

$$\vec{E}_{ext} = \vec{E}_0 - \alpha E_0\left[-2\frac{\cos\theta}{r^3}\vec{u}_r - \frac{\sin\theta}{r^3}\vec{u}_\theta\right]$$

The expression is valid for $r \geq R$ (outside the sphere). α is the polarisability of the sphere given by $\alpha = 4\pi R^3 \frac{\varepsilon-\varepsilon_{vide}}{\varepsilon+2\varepsilon_{vide}}$

1. Recall how cylindrical coordinates are defined .
[Reproduce the figure and indicate in particular the direction vectors $\boldsymbol{u}_r$and $\boldsymbol{u}_\theta$ for a point M located at the distance *r* from the center of the sphere. Indicate the angle θ].

2. Calculate the expression of the electric field $E_{ext}(A)$ at point A. Make the numerical application by expressing $E_{ext}(A)$ as a function of E_0.

3. Same question for point B.

4. Conclude on the nano-antenna effect of nanoparticles.

Numerical data : here we consider the dielectric permittivity of gold ε_{Au} = -10 à 500 nm.

APPENDIX 1. Band diagram of GaAs

Exercise I (this scheme should be included in your copy).