Exam of molecular electronics
Nov. 7, 2017

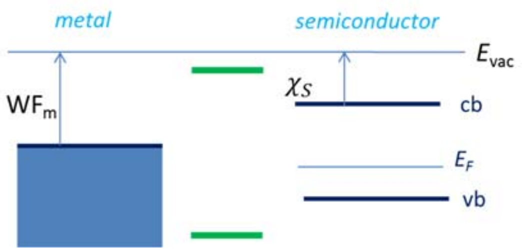
Duration: 2 hours. 1 point per question.

I. Fundamental understanding

1. Molecules of methane, ethylene and acetylene. They are hybridized sp, sp^2 and sp^3. Make the correspondence between the molecule and the degree of hybridization. Explain how hybridization explains the geometries of the molecules.
2. What does LUMO and HOMO stand for? Explain the concepts.
3. What does it mean that silicon is p-doped with a concentration of impurities of $1x10^{16}$ cm^{-3}? What are the majority carriers?
4. For an n-doped semiconductor, write the expression of the concentration of the majority carriers in the conduction band, n_c.
5. What does it mean that a p-n junction has rectifying behavior?
6. Draw the density of states as a function of energy of a quasi two dimensional system (2DEG)

II. MIS structure

Consider the following Metal Insulator Semiconductor structure when the three elements are not contacted.



1. Give the names and definitions of the various quantities indicated on this sketch
2. When the three elements are in contact, draw the band diagram at equilibrium. In particular, explain where electrons or holes accumulate, how the electric potential is modified by these charges and how it influences the energy diagram.

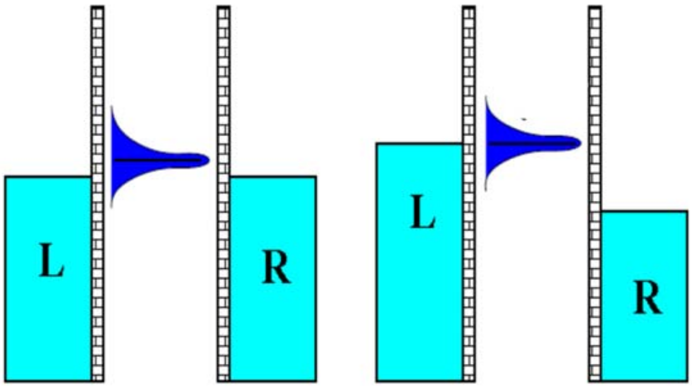
III. Coulomb Blockade

1. Explain what is meant by the term Coulomb blockade.
2. Draw the current-voltage characteristics of a single-electron transistor with a metallic island
3. Assume the island is a sphere with diameter 5 nm. What is the maximum temperature at which Coulomb blockade can be observed? The capacitance of a sphere can be calculated with the following formula: $C = 4\pi\varepsilon_0 r$.

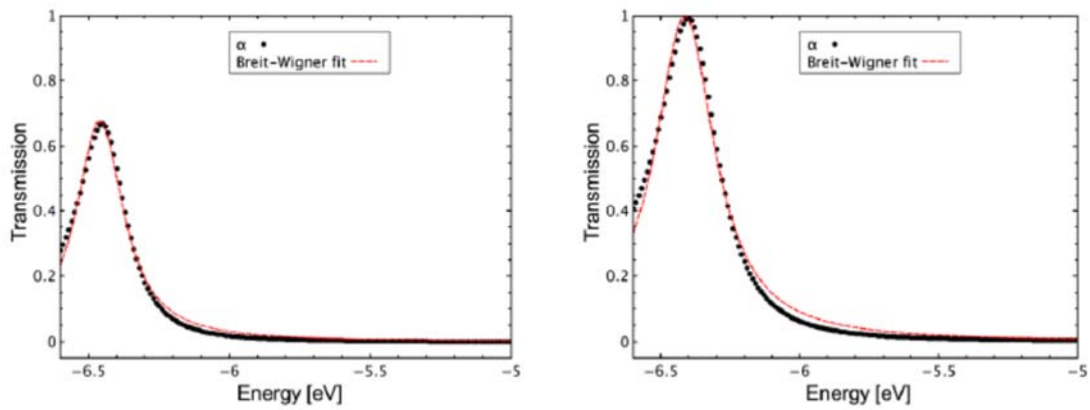
IV. Molecular conductance

Consider a molecule contacted to two electrodes L and R (for left and right).

1. Which properties determine the conductance of this single molecule contact? More specifically, explain how the concept of resonant tunneling is used for describing molecular conductance.
2. Mark the quantities Γ, E_0, E_F, eV in the drawing below. For simplicity assume symmetric coupling



3. What is the physical meaning of these quantities mentioned above in the transmission function T(E)? Give the analytic expression for T(E) in this case.



4. What is the reason why the maximum transmission in the left image is lower than in the right image?
5. Consider the right panel graph and assume a Fermi energy of E_F = -6.1 eV. How large would be the conductance of such a system at T = 0 K (right graph)?
6. Draw qualitatively the current-voltage characteristics of such a system at T =0 K! Indicate at which voltage the current increases and the approximate current scale.

V. Design an OLED

1. Explain the working principles of an Organic Light Emitting Device. Draw the band diagram for such an OLED.
2. Define the hole injection barrier and the electron injection barrier.
3. We would like to fabricate an OLED that is able to emit green light. For this device, we chose to use as emitting layer, the **Alq3** molecule (abbreviation for Tris-(8-hydroxyquinoline)aluminum). Using **Appendix 1**, explain why **Alq3** is going to emit green photons.

4. Using the data given in the **Appendix 2**, propose two well suited metals for the two electrodes. We suppose that it is possible to use these materials without creating interface states, surface dipoles or hybridizations.
5. In **Appendix 1**, the Commercial Engineers from Sigma-Aldrich propose a more complex structure for an OLED made of **Alq3**. Give two reasons why they propose such a structure (there are more than two reasons…).

Values of natural constants:

Vacuum permittivity $\varepsilon_0 = 8.854\times10^{-12}$ F/m
Boltzmann constant $k_B = 1.381\times10^{-23}$ J/K
Elementary charge: $e = 1.602 \times 10^{-19}$ C
Free electron's mass $m = 9.109\times10^{-31}$ kg
Planck's constant $h = 6.626\times10^{-34}$ Js
Speed of light· $c = 2.999 \times 10^{8}$ m/s

APPPENDICES

APPENDIX 1. Data on Alq3 [Tris-(8-hydroxyquinoline)aluminum] from Sigma-Aldrich catalog

Downloaded on 21-nov-2016: https://www.sigmaaldrich.com/

444561	Tris-(8-hydroxyquinoline)aluminum, 99.995% trace metals basis,	ITO/MoO_3/NPD/Alq_3/BPhen/LiF/Al • Color: green • Max. Luminance: 20000 Cd/m² • Max. EQE: 1.2 % • Turn-On Voltage: 2.8 V	LUMO -3.3 eV HOMO -5.8 eV	

Conditionnement - SKU	Disponibilité	Prix (EUR)
444561-1G	**Disponible pour expédition le 21.11.16 - A PARTIR DE**	**62.30**
444561-5G	**Seulement 5 en stock (d'autres en cours d'arrivage) - A PARTIR DE**	**210.00**

APPENDIX 2. Work function of metal electrodes.

Sze, *Physics of Semiconductor Devices*. p 366.

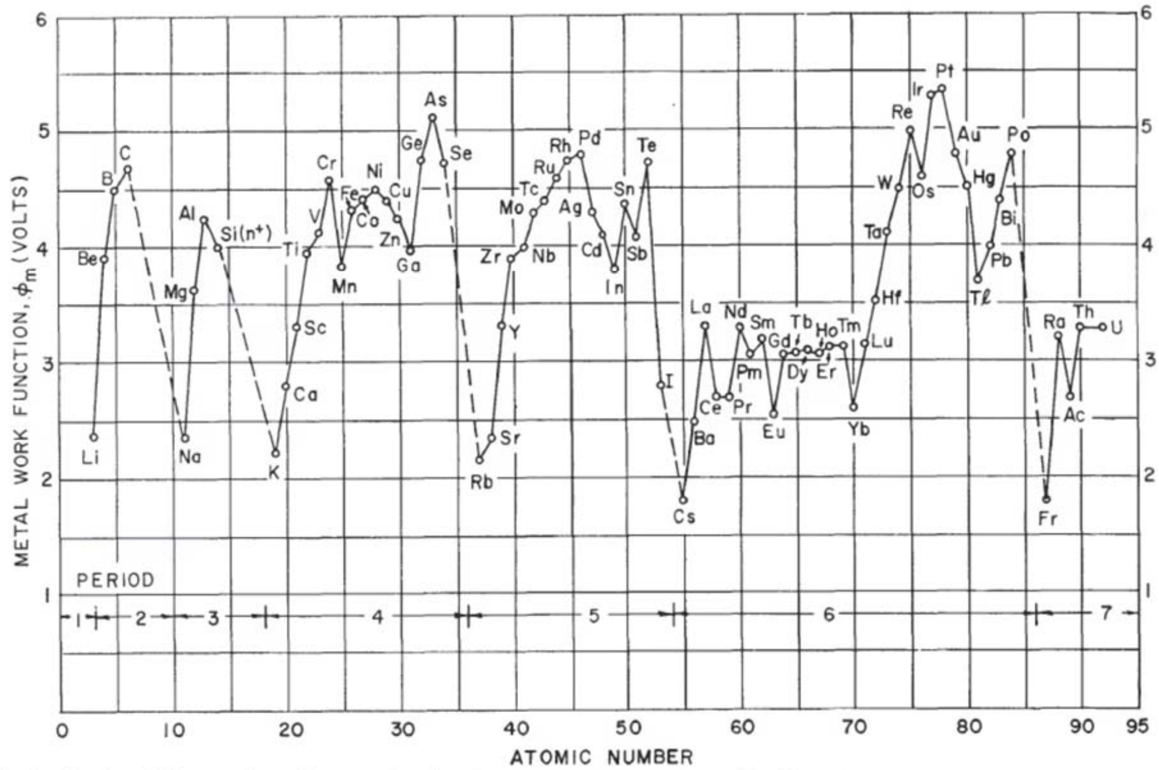


Fig. 2 Metal work function for a clean metal surface in a vacuum versus atomic number. Note the periodic nature of the increase and decrease of the work functions within each group. (After Formenko, Ref. 7.)