NanoElectronics Exam 30 January 2012
Course code: 193400141

> ***Important:*** *This exam consists of **4 problems**, worth **100 points** in total. The maximum number of points you can get for each question is indicated. Write down your name on each sheet of paper that you hand in. Make each problem on a separate sheet (or separate sheets).* ***The exam you are about to enjoy is a <u>closed-book exam</u>, i.e. study material of any kind is <u>not</u> allowed during the exam.***

list of physical constants:

Planck constant $\qquad h = 6.6260755 \cdot 10^{-34}$ J·s
Boltzmann constant $\qquad k = 1.380658 \cdot 10^{-23}$ J·K^{-1}
Elementary charge $\qquad e = 1.60217733 \cdot 10^{-19}$ C
Permeability of vacuum $\quad \mu_0 = 4\pi \cdot 10^{-7}$ T·m·A^{-1}
Bohr magneton $\qquad \mu_B = 9.2740154 \cdot 10^{-24}$ J·T^{-1} [T=J·A^{-1}·m^{-2}]

PROBLEM 1: General Aspects (25 points)

Below, several statements are given. Indicate for each statement whether it is **true** or **false**, and **motivate your answer**.

1A (3 points)
Consider a crystalline organic semiconductor with the (calculated) band structure shown below.
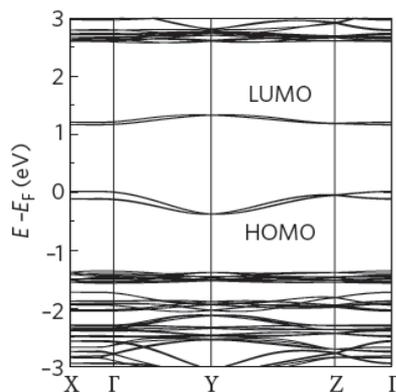
Calculated band structure of a rubrene crystal. The energy (E) is plotted vertically, the wave number (k) runs horizontally, along certain high symmetry directions (the symmetry points are labeled Γ, Y, Z, etc.).

Statement: the electron mobility is higher than the hole mobility along the Γ→Y direction in this crystal.

False. The effective mass is inversely proportional to the curvature (the second derivative of E(k), $\partial^2 E/\partial k^2$), of the bands. Electrons go into the LUMO-derived band, for which the curvature is considerably smaller than that of the HOMO-derived band, containing the holes. Therefore the electron effective mass is higher than the hole effective mass, leading to a higher velocity of holes in the material. The mobility is defined as the ratio between the carrier drift velocity and the electric field; the hole mobility is thus higher than the electron mobility.

1B (2 points)
Hopping conduction can occur even in completely defect-free organic single crystals.

True. Charges can become trapped by geometrical relaxation of the molecules in the crystal. For insufficiently large band-widths, the average residence time of carriers on individual molecules will be longer than the geometrical relaxation time of about 10^{-14} s. In this case, the charged molecules relax their energy by assuming a new geometry, thus trapping the carrier. Transport then proceeds via hopping.

1C (3 points)
The (time averaged) amount of electrons on a molecule in a single-molecule transistor is mainly determined by the source-drain voltage.

False. The amount of electrons on the molecule depends mainly on the gate voltage, which pulls/pushes the electronic energy levels of the molecule down/up relative to the Fermi level of the source/drain electrodes. When a certain molecular energy level is pulled (pushed) below (above) the Fermi level of the source/drain leads, it becomes filled (empty). The source-drain voltage determines the current flow through the transistor.

1D (2 points)
The LUMO wave function of a π-conjugated organic molecule has exactly one more zero crossing than the HOMO wave function.

True. For each consecutive energy eigenvalue, another node (zero crossing) appears in the wave function. This is most easily seen for particle-in-a-box wave functions, but also holds for atoms (e.g. 1s, 2p, 3d wave functions) molecules, and solids. The HOMO and LUMO levels are states of consecutive energy eigenvalues (there is no other state in between), such that the LUMO contains one additional node.

1E (3 points)
The spin polarization of the current flowing through a ferromagnetic metal is directly proportional to the spin polarization of the density of states at the Fermi energy.

False. Not all states contribute equally to the current flow, *e.g.* in 3d transition metal ferromagnets the s-electrons carry the current while the d-electrons are relatively immobile. The spin polarization of the current is therefore not directly proportional to the spin polarization of the DOS; a partial DOS has to be considered.

1F (2 points)
In a hypothetical material for which the spin-orbit coupling is zero, the spin lifetime must be infinite.

False. Carrier spins can relax/dephase also via interactions with nuclear spins (hyperfine interaction).

1G (3 points)
The exchange interaction can result in parallel as well as antiparallel alignment of electron spins on neighboring atoms.

True. The exchange interaction is related to the requirement that a multi-electron wave function must be antisymmetric upon exchange of any pair of electrons. This imposes that when the spin-dependent part of the wave function is antisymmetric

under exchange (antiparallel alignment of spins), the position-dependent part is symmetric, and vice versa. Whether an antisymmetric or symmetric position dependent part is favored depends on the relative positions of the nuclei and the extension of the electron clouds, both situations can (and do) occur.

1H (2 points)

The magnetic field **B** and the auxiliary magnetic field **H**, related via $\mathbf{B}=\mu_0(\mathbf{H}+\mathbf{M})$ where **M** is the magnetization vector, always point in the same direction.

False. Inside a ferromagnetic material, **H** is opposite to **M** and **B**. The **H**-field, or auxiliary magnetic field, originates and terminates at the surface-poles of a ferromagnet, thus acting to demagnetize it. For this reason, it is also called "demagnetizing field".

1I (3 points)

The domain walls in a ferromagnet with a large magnetocrystalline anisotropy constant are wider than in an otherwise similar ferromagnet with a small magnetocrystalline anisotropy constant.

False. Inside a domain wall, the magnetization rotates, such that it cannot always point along the magnetic easy axis. For materials with a large magnetocrystalline anisotropy constant, the energy penalty associated with this is also large. This tends to make the domain walls narrower, not wider.

1J (2 points)

Magnetic nanoparticles for which the anisotropy constant is large have a higher thermal stability (longer magnetization reversal time) than similar nanoparticles with a small anisotropy constant.

True. A large anisotropy constant opposes random fluctuations of the magnetization. The anisotropy energy forms a barrier that the system has to surmount via thermal excitation in order to change its magnetization.

PROBLEM 2: Organic electronics (25 points)

2A (4 points)
Consider a tetracene crystal, with a molecular packing configuration as shown below. The arrows indicate two possible directions for charge carrier transport. In which direction, running vertically or horizontally in the figure, do you expect that the charge transport is faster? Motivate your answer!
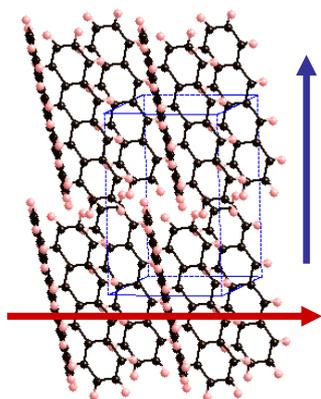
The charge transport is fastest in directions along which the wave-function overlap is largest. The relevant orbitals are the HOMO (hole transport) and LUMO (electron transport) of tetracene, which are both π-orbitals that extend away from the molecular plane, i.e. in the direction of the horizontal arrow in the figure. Therefore, the transport is fasted along the horizontal direction.

2B (5 points)
Tetracene thin films can grow in several different crystal phases, featuring different packing modes of the molecules. Do you expect that the hopping rates for holes will be different in these different films? If so, is this due to different reorganization energies, or different transfer integrals? Motivate your answer!

Indeed the hopping rates depend on the packing of the molecules in the films. The reorganization energy arises from the distortion of the geometry of the tetracene molecule upon charging it, thus a change in the position of the carbon and hydrogen nuclei that make up the molecule when electrons are added/removed. This is not significantly affected by the environment. The transfer integrals, however, strongly depend on the wave function overlap between neighboring molecules, and thus on the packing mode.

2C (5 points)
Assume that the geometrical relaxation time of a tetracene molecule is on the order of 10^{-14} s. Give a rough estimate of the minimum value of the HOMO band-width that would result in band-like motion. What is the relation between the band width and the corresponding transfer integral?

The band width W that would result in a residence time τ about equal to the geometrical relaxation time can be estimated from the Heisenberg uncertainty relation $W\tau > \hbar$. This gives $W \approx 10^{-20}$ J, or $W \approx 0.1$ eV. The transfer integral for the orbitals on

neighboring molecules that make up the band with width W is, as a rule of thumb, about 4 times smaller than that.

2D (6 points)

Consider a tetracene thin film transistor, as shown schematically below. Discuss the operation principles of such a transistor, as precisely as possible. What happens in the saturation regime?
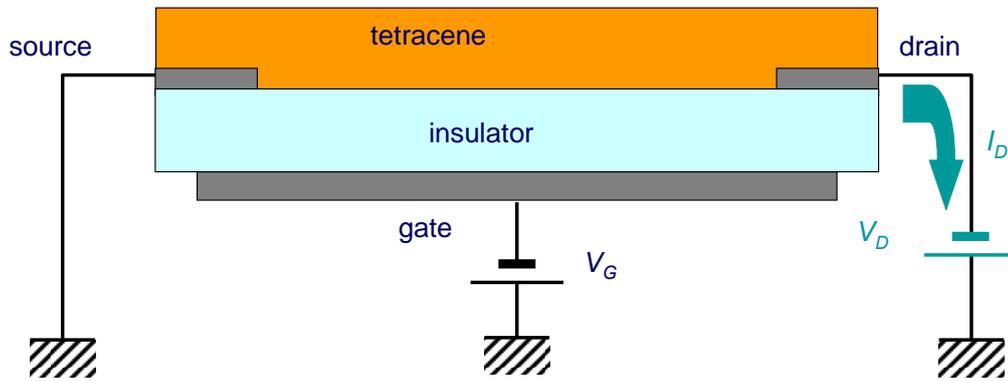

An organic thin film transistor (OTFT) behaves as a capacitor, where one plate is constituted by the gate electrode, and the other one by the semiconductor film. When a voltage V_G is applied between source and gate, charge carriers accumulate at the insulator-semiconductor interface, leading to the formation of a conduction channel between source and drain. A high accumulated charge density at the insulator/organic semiconductor interface leads to a high source-drain current when a voltage V_D is applied. The saturation regime is reached when the source-drain voltage V_D becomes equal to the (source-)gate voltage. There is no potential drop between drain and gate anymore, which destroys the charge accumulation close to the gate. The conduction channel is interrupted, or "pinched off".

2E (5 points)

Sketch the drain current, I_D, versus drain voltage, V_D between 0 and 80 V, at a fixed gate voltage, $V_G = 40$ V, and identify the different operation regimes. How can we determine the charge carrier mobility from such a plot?

Arrows indicate when V_G is about equal to V_{SD}; this is the point at which saturation sets in
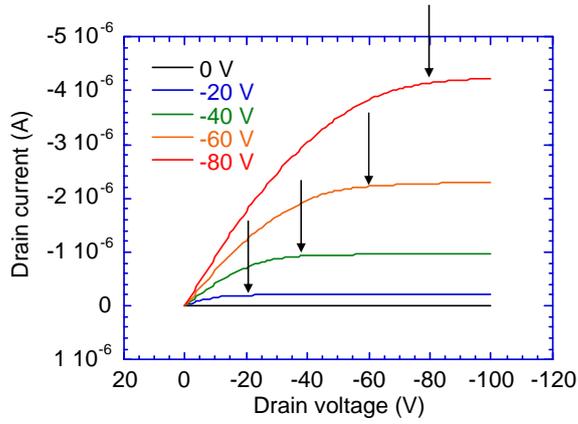
$$I_D = \frac{W}{L} C_i \mu (V_G - V_T) V_D$$

W and *L* = channel width and length
C_i = capacitance of the insulator layer
μ = mobility
V_T = threshold voltage (accounts for voltage drops of various origin across the insulator-semiconductor interface)

PROBLEM 3: GMR, TMR and spin transfer torque (25 points)

3A (5 points)
Using the figure below, explain why the resistance for majority spin electrons, R_{maj}, and the resistance for minority spin electrons, R_{min}, is different in Co.
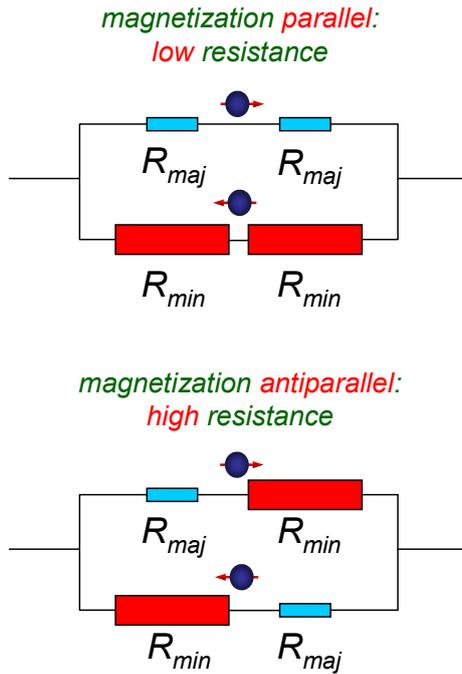
As the figure shows, the DOS at the Fermi energy, where the mobile electrons reside, is very different for majority *vs* minority spin electrons. There are no spiky majority *d*-bands at the Fermi level, while such states *are* present in the minority DOS. Assuming that the spin is conserved upon scattering, the mobile minority s-electrons can scatter into these states, but the majority s-electrons cannot. This leads to different scattering rates of minority/majority electrons (high/low scattering rate) and thus also a different resistance.
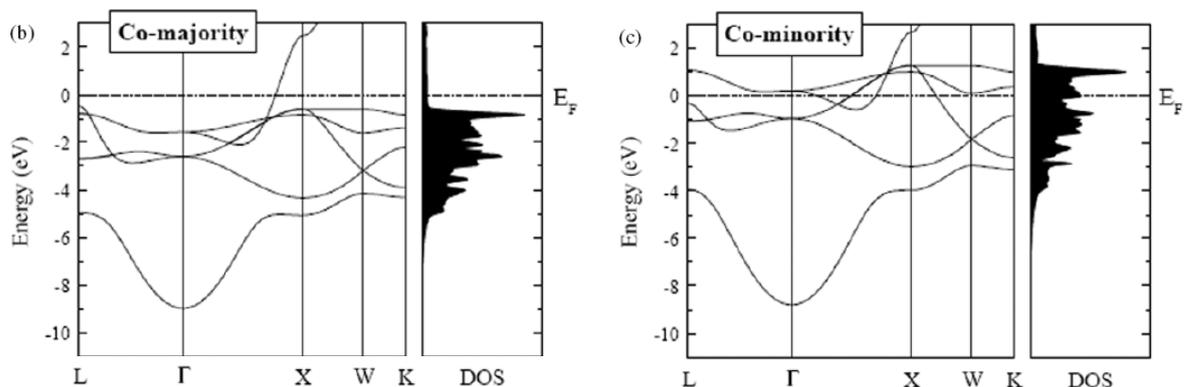
Now consider a Co/Cu/Co spin-valve, consisting of two thin Co layers separated by an ultrathin Cu spacer layer of a few nanometers thick (the magnetization of one of the Co layers is somehow kept fixed).

3B (5 points)
Sketch a spin dependent resistor network that "models" the electrical resistance for current flow through the Co/Cu/Co stack, for two different cases: i) Co layers magnetized parallel, ii) Co layers magnetized antiparallel. You should neglect spin-flip scattering, such that the two current model of N.F. Mott applies. The resistance of the Cu spacer can also be neglected.

magnetization parallel:
low resistance

R_{maj} R_{maj}

R_{min} R_{min}

magnetization antiparallel:
high resistance

R_{maj} R_{min}

R_{min} R_{maj}

3C (5 points)

Explain why the Cu spacer layer should be very thin, only a few nm, to attain a robust GMR. To which characteristic length should the spacer thickness be compared?

The spacer layer should be thin enough to allow the electrons to pass through easily, e.g. without being scattered. It should thus be thinner than the electron mean free path.

Now consider a $Co/Al_2O_3/NiFe$ magnetic tunnel junction (MTJ). The magnetic hysteresis loops of the Co and NiFe layers are shown in the picture below.
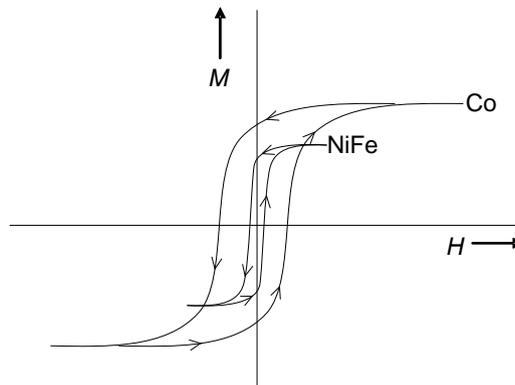
3D (5 points)

Sketch the resistance of the MTJ versus the magnetic field, when the field is swept from a large negative value to a large positive value and back. Explain your drawing. Also explain how the MTJ can be used as a memory element.
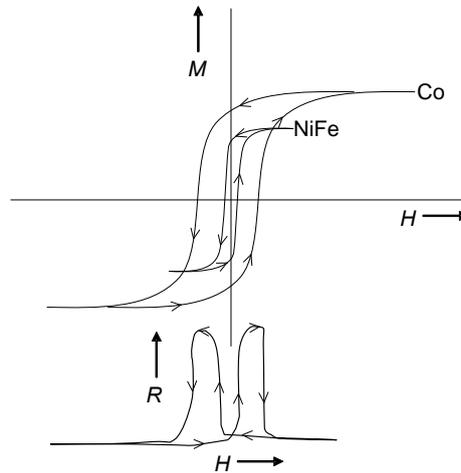
Resistance increases abruptly as the NiFe layer reverses its magnetization when the field is swept through zero (layers magnetized antiparallel), then switches back to the low value when also the Co layer switches (parallel magnetization). The low resistance state may serve as "0" and the high resistance state as "1" in a memory element.

3E (5 points)
What is meant by spin transfer torque? Explain the benefits of switching MTJs with spin transfer torque as compared to magnetic field induced switching in conventional magnetic random access memory.

Spin transfer torque is the torque on the magnetization vector of a ferromagnetic element resulting from a spin polarized current flowing through it, where the spin polarization vector is non-collinear with the magnetization vector. If the current density is large enough, this may lead to (continuous) rotation or reversal of the magnetization of the FM element. Switching MTJs using spin transfer torque has great benefits for the (down) scaling of magnetic memory, which is hampered in conventional magnetic memories that operate by magnetic field (generated by currents through a wire-mesh) induced switching due to cross-talk between bits when the bit size is decreased. Spin transfer torque switching does not suffer as the bit size shrinks, in fact it becomes easier to switch smaller magnetic elements with STT!

PROBLEM 4: Inorganic nanoelectronics (25 points)

The conductance quantum e^2/h plays a fundamental role in inorganic nanoelectronics. Not only does it appear in quantized conductance, but also in the Aharonov-Bohm effect and in Coulomb blockade.

The **bold** words indicate the necessary input to get the point

4A (7 points)
Explain how the conductance quantum *appears* in the quantization of conductance through a quantum point contact (QPC). Describe features qualitatively and quantitatively.

The conductance through a QPC equals $\mathbf{G = N_{max}*2e^2/h}$. (2)
A gate voltage can control the number of modes through the QPC, resulting in **steps in the conductance** versus gate voltage (2)
Every **mode/channel/subband** adds 2 units of conductance e^2/h. (1)
The doubling of the conductance quantum is a result of **spin degeneracy**: every mode has a spin-up and spin-down channel which both contribute e^2/h. (1)
A finite **magnetic field lifts the spin degeneracy**, resulting in steps of e^2/h instead of $2\ e^2/h$ (1).

4B (5 points)
Explain how the conductance quantum *appears* in the Ahoronov-Bohm effect. What is required with regards to the phase coherence length? How does the size of system influence the effect?

The conductance through an AB ring oscillates as $G = G_0 + G_{AB}$ with $\mathbf{G_{AB} \sim e^2/h\cdot cos}$ $(2\pi\Phi/\Phi_0)exp(-L/l_\varphi)$ (1).
The oscillations are a result of **quantum interference** of electron waves as they propagate through the ring. (1)
The phase coherence length $\mathbf{l_\varphi}$ **must be longer than the circumference of the ring L**. for the quantum interference to occur, see the equation above: G_{AB} falls off exponentially with L/l_φ. (1).
The conductance thus oscillates with magnetic field, where the period is determined by the area of the ring as T = $\mathbf{\Phi_0 = h/e}$. Note: this is a flux quantum, not a conductance quantum. (1)
The area of the ring determines the period in B field: $T = \Phi_0$. For a ring of area A ($=L^2/4\pi$), we get the period in B from BA = h/e; $S = \pi r^2$, ==> $B = h/Ae = 4\pi h/L^2 e$ (1)

4C (3 points)
Explain how the resistance quantum is relevant to observe Coulomb blockade. What are the requirements to observe Coulomb blockade?

Uncertainty principle ==> $R > h/e^2$.

4D (5 points)
There are two energy scales that determine electron transport through quantum dots. One of them is the charging energy, given by e^2/C. Explain carefully what the charging energy is and what the symbol C stands for in this expression? Also, how

large should this charging energy be to measure single-electron charging effects at room temperature?

The charging energy is the energy required to add the charge of 1 electron e to the island of a single-electron transistor or QD. C is the total capacitance of the island, which is the sum of the capacitance of ALL gates to the dot. In the simplest picture there are three contributions: C_S, C_D, and C_G. C then equals $C = C_S + C_D + C_G$.

$E_C > k_BT$. Otherwise the thermal energy would facilitate transport At RT, $k_BT =$ 1.38E-23*300/1.6E-19 ~ 26 mV, so $E_C > 26$ mV.

4E (5 points)
The other energy scale that determines electron transport through quantum dots, we refer to as the orbital level spacing ΔE. What determines the magnitude of the orbital level spacing?

$\Delta E \sim h/m^*L^2$, so always m^* (depends on crystal) and size L. Furthermore the confinement potential is important. In case of a hard-wall potential, ΔE increases with electron number N. In case of a harmonic oscillator potential, ΔE is independent of electron number, but the finite well height influences ΔE.

END OF EXAM