Material Physics Exam Jan 24 questions

~~Explain Fermi level Pinning and its impact on the Schottky Barrier~~

* Explain the electronic structure of conjugated molecules and ways to improve it

Conjugated molecules: it is originated from the alternating multiple/single bond because of the shift of the charge. **Pi-bonding between sp2 C atoms results in delocalized MOs.** Called the **resonance bonding.**

Benzene: the pi bonds result from overlap between two orbitals. The pi-pi stacking comes from the overlap of pi bonds. **This is the result of hybridization.**

Energy structure: the delocalization of the pi bonds, the electron can move in the molecular pi bonds stuck at the sigma bonds. The Huckel’s method tells us the linear combination of the entire molecule and introduce the LUMO and HUMO. For butadiene, it’s still able to use this method while the HOMO and LUMO are different from different configuration like bonding and antibonding. And with more C atom in the whole system, the bandgap will decrease.

Way to improve it: 1. We can play with the twist angle of two molecules, twist reduce pi-orbital overlap leads to bandgap increases 2. We can use heteroatoms with different electronegativity to modify the bandgap, overlap more, the lower the bandgap, easier to electron to move around. 3. Electrons from homo are more easily trap by the impurity, make the molecule more unstable since the lowering the energy is more easily. That requires the material to have smaller bandgap. While there is another unstable factor comes from the air (wet oxygenation) if ionized potential is less than 4.9eV, so p-type material with low HOMO is more stable. That means the tricks like withdrawing groups are needed to lower the HOMO. All in all, low LUMO and low HOMO devices are more favored according to its good stability.

~~Explain the electronic transport in graphene~~

* Discuss size effects in magnetic materials

The size effects play an important role. When the volume drops below a certain critical value, it becomes energetically unfavorable to include a domain wall, and the uniformly magnetized state becomes the lowest energy configuration.

There is somewhat the temperature below the Curie temperature, because the magnetization is related to the volume and its barrier is the in the mid of the easy axis. However, if the thermal fluctuation goes up, the magnetization direction would flip with the same magnetization level can reach. The Neel relaxation indicates the possibility for the material to flip, indicates the possibility for the bulky material is almost impossible.

Size effect on coercivity: after the size crystallite size increases and jump away from the superparamagnetic region, the coercivity will gradually reach the maximal and the critical size. However, if this becomes the multi-domain, then the H apply with more likely to move the domain walls, that decrease the ability to be a hard magnet.

* Explain heterojunctions. Their nature, band bending and applications

Fermi levels will be equal between two heterojunction devices, with different Eg the bending would make some difference. We can use voltage to tune the band structures. From the normal Si device, we can have the unsymmetric valence band and conduction band. When p51 indicates that the barrier against electron diffusion is much lower than the barrier against the hole injection. Therefore, the electron and holes flow differently.

HBT: the dissymmetry of energy band discontinuities at the emitter/base interface is such that the electron diffusion current from the emitter to the base is higher than the hole diffusion current from the base to the emitter.

HEMT: skip see the answers sheet

~~How to use Er-doped fibers in amplifiers~~

~~Temperature-dependence in ferro-electric materials (phase transition)~~

* The origins of magnetism

It’s from the electron spin, while up and down indicate the north pole and south pole. This is made by Hund’s rule. The spin imbalance will maximize the total spin, this is how the original of the magnetism. In case there is equal number of electrons with spin up and down, this is diamagnetic. Otherwise, it could be ferromagnetic.

If we look at in the molecule status, the exchange energy indicates the overlapping with the electronic orbitals j and i. And the we trying to make the energy always at the lowest value and found the antiferromagnetic and ferromagnetic.

* Discuss piezo, ferro and pyro electrics, what are the differences and similarities?

Piezoelectricity:

Definition: Piezoelectric materials generate an electric charge or voltage across two sides of the material when mechanical stress (pressure, bending, etc.) is applied. Conversely, they can change shape when an electric field is applied.

Example: Quartz, certain ceramics like Lead Zirconate Titanate (PZT).

Ferroelectricity:

Definition: Ferroelectric materials exhibit a spontaneous electric polarization (an inherent electric field) that can be reversed by the application of an external electric field. This polarization is not only responsive to electric fields but also stable and switchable, which distinguishes them from other materials.

Example: Barium Titanate, PZT (also piezoelectric).

Pyroelectricity:

Definition: Pyroelectric materials generate a temporary voltage when they are heated or cooled, which changes their temperature. This effect is due to a change in the polarization of the material due to temperature variation.

Example: Tourmaline, Lithium Tantalate.

**Similarities:**

Polarization: All three types of materials exhibit some form of polarization. Piezoelectrics and ferroelectrics can have their polarization altered by mechanical stress or electric fields, respectively. Pyroelectrics have a polarization that changes with temperature changes.

Material Overlap: Some materials can exhibit more than one of these properties. For example, PZT is both piezoelectric and ferroelectric.

Applications: All are used in sensors and actuators, leveraging their ability to convert mechanical, thermal, or electrical energy from one form to another.

**Differences:**

Cause of Polarization:

Piezoelectricity arises from mechanical deformation.

Ferroelectricity is related to the structure of the material which allows for a reversible spontaneous polarization under an electric field.

Pyroelectricity is caused by changes in temperature affecting the polarization.

Reversibility:

Piezoelectrics and ferroelectrics exhibit reversible changes (mechanical to electrical and vice versa for piezoelectrics; electrical polarization direction changes for ferroelectrics).

Pyroelectricity involves a temporary change that occurs only during temperature change and will return to its original state once the temperature stabilizes.

Dependency:

Piezoelectric effects are dependent on the mechanical stress applied.

Ferroelectric effects depend on the history of the electric field application (hysteresis behavior).

Pyroelectric effects are solely dependent on temperature changes.

* Explain the electronic properties of CNT

The chiral directions are crucial for the CNT while (n,m) indices thus defines the diameter of the CNT. Could be Armchair, zig-zag. And statically there will be 1/3 metallic and 2/3 semiconducting… (skip the following, just follow the slides)

~~What is Seebeck coefficient? What are the parameters affecting Seebeck coefficient? Describe strategies to increase it.~~

* Explain how to engineer the bandgap of graphene.

Some about the GFET, skip….

**Symmetry breaking:** For the bilayer, we can have two symmetries breaking while the inversion changes the the bandgap structure.

**Quantum confinement:** Or we can do is specify the direction of the graphene, that helps us to have zig-zag ribbon and construct special bandgap.

~~Explain the carrier concentration in intrinsic semiconductors. Explain the temperature dependence of it in device's properties.~~

~~Discuss the two models for conductivity in metal. What are their main differences?~~

* How can I have a high efficiency LED?

For making a LED we need a direct bangdap without k-value.

Photon emission occurs whenever we inject minority carriers recombining with the majority carriers. The recombination is going to happen in the depletion region. The electron diffusion length is greater than the hole diffusion length, the phonon emitting region will be larger on the p-side of the junction rather than n-side. That means small depletion width at the n++ region and large depletion on the p-side.

There is quantum yield happens for a LED, that might be the reflection of the surface.

* How to increase the efficiency of lasers?

Make a cavity, one is partially transparent, and one is completely reflective.

Make use of the heterojunction, electrons are confined in the mid active region that make the recombination more easy to happens.

~~Discuss what defines the thickness of magnetic domain walls.~~

~~Discuss the resistivity and scattering in metallic thin films and polycrystalline materials.~~

~~How do LCAOs lead to band structures in crystals.~~

* Explain the doping process for PEDOT:PSS

The C(N) doping as a secondary doping could form a nanofiber mythology. That’s distorted original pan-cake structure. While with the addition of the SD, the doping concentration will be decreases and change carrier transportation between the layers of PEDOT:PSS.

Specify the change: Benzoid-rich and Quinoid-rich system has forced the planar molecule arrangement into distorted one. The bigger the C(N), the larger the distance will be. Page 90 is telling the C(6) and C(13) are more efficient for the dedoping. Since the bipolaron is induced via doping.

That means we can play with that and use dedoping to have a wanted organic thermoelectric device.

~~What are the limitations of graphene FET and what are the alternatives~~

~~Effective mass approximation for semiconductors~~

* Explain how STT-MRAM works and its advantages compared with standard MRAM

Normally, we need use current that can magnetized the MRAM bit to store the data on it. However, this method consume too much energy and too slow.

The STT-MARM make uses of the spin torque of the current that can change the magnetization direction. Then the direction would change immediately.

~~Explain the function of bulk heterojunction for organic solar cells~~

* How is white light produced?

First we need to find that the red one and green one and these two are relatively easy

The blue one is hard to find, but finally find it in the end. Then combine them with a certain ratio will give a white color.