School of Engineering
Institute of Materials
Laboratory of Macromolecular
and Organic Materials

# Organic Electronic Materials 2025 Exercise 1 Solutions

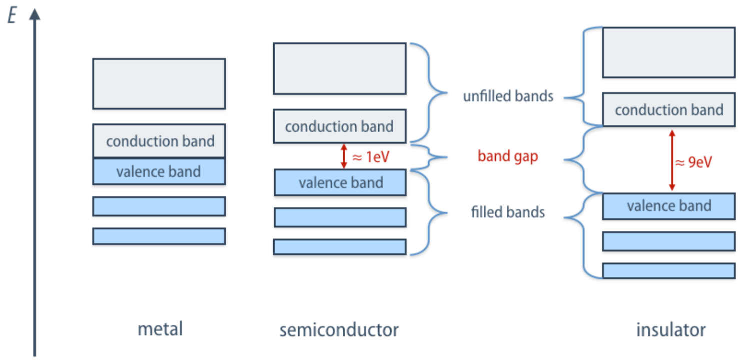
## *Solutions*

1. What is the difference between a metal, a semiconductor, and an insulator? Illustrate your answer. Explain the consequence of this difference on their conductivity and clarify the distinction between conductivity and mobility.

*A metal is a material where there is no gap between the highest occupied energy level and the lowest unoccupied one at the absolute zero temperature, so with even some energy, electrons are free, as they can readily hop on the conduction band, which is a parameter towards efficient conductivity.*

*On the other hand, insulators are defined as material in which there can be no flow of electric current. Such materials generally have a large band gap between the conduction band and valence band, so that even when given high energy, the valence band remains full and the conduction band empty.*

*Semiconductors have a smaller band gap than insulators allowing them to get some electrons on their conduction band and a partially empty valence band, under the influence of electric field, increased temperature, or light interaction. Therefore, some conductivity can be observed.*




*The mobility of charge carriers in a material corresponds to how quickly those charge carriers can move in the material.*

*The conductivity of material defined as $\sigma = n * e * \mu$ with $\mu$ the mobility and $n$ the density of charges, indicates the ability of a material to conduct an electric current.*

2. Give the time-independent Schrödinger equation in its most general form, briefly name/define all parameters/variables that appear in it and paraphrase the meaning of the Schrödinger equation. Why is it actually a differential equation?

$$\hat{H}\psi = E\psi$$

*Schrödinger equation is a differential equation that describes the allowed states (stationary state wave functions ψ) of an electron in quantum system.*

*H Hamilton operator, set of operations that describes the total energy of the quantum system*

*E is the energy associated to the stationary state wave function ψ, ie the eigenvalue of the Schrödinger equation associated to the eigenvector ψ.*

*The Schrödinger equation is a differential equation because the unknow is a function (not a fixed numerical value) and, derivatives are among the operations inside the Hamiltonian operator, therefore, the Schrödinger equation relates a function to its derivative.*

3. What is an atomic orbital? Explain how it is graphically represented.

*An atomic orbital is the spin-independent term of a wavefunction solution of the Schrödinger equation for an atomic system. It is a complex function of space giving the allowed position of an electron at the associated energy. It is graphically represented by an isosurface of the probability density* $(|\psi\rangle($^{2}$ = const$.

4. What is the valence shell? Why are noble gases particularly stable?

*The valence shell is the outermost/highest energy shell (shell are set of orbitals defined by a principal quantum number) plus eventually incomplete subshells. The electrons in the valence shell are called valence electrons and are the ones that can participate in chemical reactions and bonding with other atoms. Noble gases are particularly stable because they have the maximum number of valence electrons in their valence shell, so they rarely react with other substances.*

5. Explain the VSEPR model. Draw and explain the structure of $H_2O$, $NH_3$, $PF_5$, $BF_3$, $SO_2$, and $CO_2$.

*The VSEPR (Valence Shell Electron Pair Repulsion) model is a theory used to predict the shapes of molecules based the number of electron pairs around the central atom, including both bonding and non-bonding electron pairs. It is based on the idea that electron pairs in the valence shell of an atom repel each other, and therefore, they tend to be arranged as far apart as possible to minimize repulsion, leading to specific molecular shapes.*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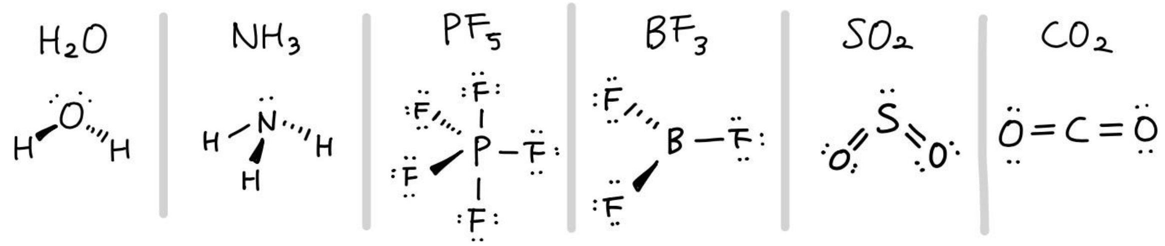



*$H_2O$ $AX_2E_2$ Bent 109.5°*

*$NH_3$ $AX_3E$ Tetrahedral*

*$PF_5$ $AX_5$ Trigonal bipyramid*

*$BF_3$ $AX_3$ Trigonal planar*

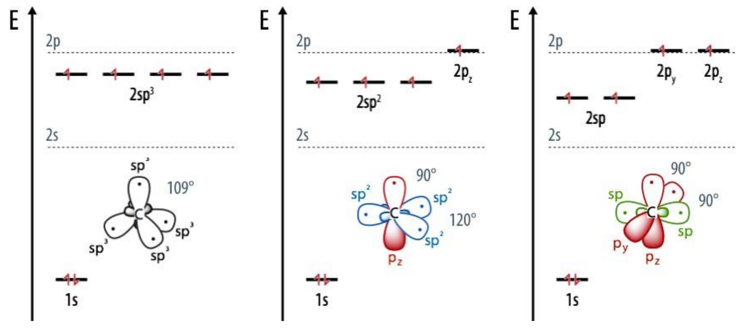
*$SO_2$ $AX_2E$ Bent 120°*

*$CO_2$ $AX_2$ Linear*

6. Explain the concept of "hybridization" of atomic orbitals and what it is useful for. Detail the case of carbon atoms in its three different states of hybridization, including AO energy level diagrams and pictorial representations of the derived hybrid AO.

*Hybridization is the concept of mixing the valence shell atomic orbitals (pure states) by linear combination to form new set of hybrid orbitals with equal energy, that are more suitable to predict and explain geometry and bonding in molecules.*

*The electron configuration of a carbon atom is $1s^2 2s^2 2p^2$. There are three different states of hybridization in the carbon atom $sp^3$, $sp^2$, and sp.*




7. The construction of hybrid orbitals and molecular orbitals both use linear combinations of atomic orbitals. Give a simple answer, what is the difference between the two?

*MOs are linear combinations of AOs of different atoms, while hybrid orbitals are linear combinations of AOs within one atom*

8. **Homework** – After reading the two articles "Progress and Challenges in Commercialization of Organic electronics" and "The Dawn of Organic Electronics", write a few sentences on each of the following questions:
   - What shortcomings are present in organic electronic devices?
   - What reasonable applications can you envision for organic electronic devices?
   - With some light research online (Google Scholar, …) try and find a recent application of organic electronics which you find interesting

**Further reading:**

*Organic Chemistry*, Clayden, Greeves & Warren 2012 – Chapter 4 – Structure of molecules (or the corresponding chapter in any other organic chemistry book)

*Physical Chemistry*, Atkins & de Paula -Chapter 8– Quantum Theory: Introduction & Principles

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