LCAO (Linear Combination of Atomic Orbitals)

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Nowadays, nanomaterials are becoming more and more popular with their various applications. Thus, it is of great importance to study and understand how things work in Nano-scale. LCAO is a well-known technique which is used to calculate molecular orbitals in quantum chemistry.

In the presentation, we are going to examine some examples about how atoms create molecules and then how molecules create solid materials under the scope of quantum mechanics. Firstly, we are going to start with Schrödinger's equation and study the basic idea of a chemical bond which is created by two atoms with symmetric and then with antisymmetric quantum well. Afterwards, we will talk about hybrid orbitals sp^1 ,sp^2,sp^3 and the example of C_6H_6. Finally we are going to expand the LCAO theory in a linear hydrocarbon chain and show how the discrete eigenenergies of electrons become continuous.

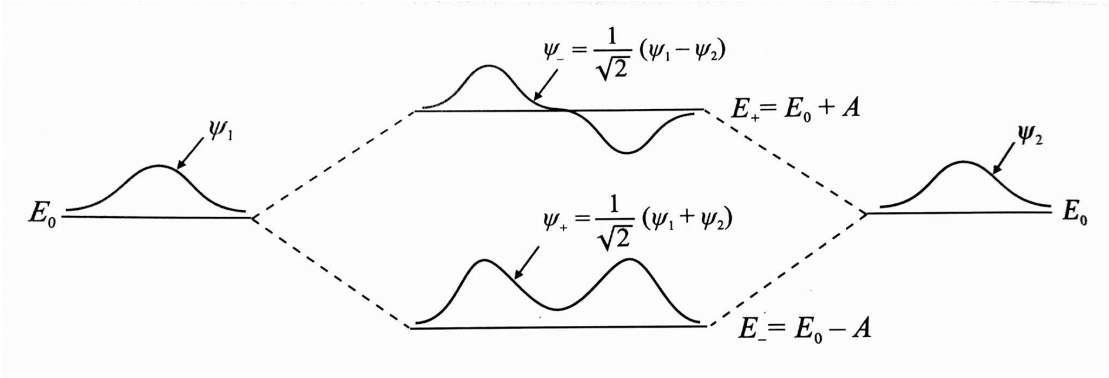

Figure 1: the eigenenergies and wavefunctions of symmetric double quantum well with LCAO .[1]

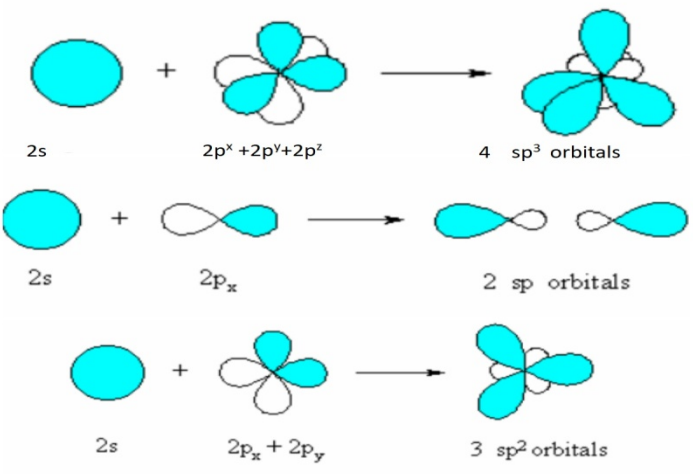

Figure 2: S + P orbitals are combined and create the hybrid orbitals sp^1 sp^2 sp^3. [3]

References

[1] Τραχανάς Σ., 2008. Κβαντομηχανική ΙΙ , Θεμελιώδεις αρχές και μέθοδοι, κβαντικοί υπολογιστές. Ηράκλειο: Πανεπιστημιακές εκδόσεις Κρήτης.

[2] Οικονόμου Ε. Ν., 2016. Επιτομή Φυσικής Στερεάς Κατάστασης. Ηράκλειο Πανεπιστημιακές εκδόσεις Κρήτης.

[3] http://www.chem.ucalgary.ca