

Fundamentals of Nanoelectronics

ECE495 - Session 15, Sept 28, 2009

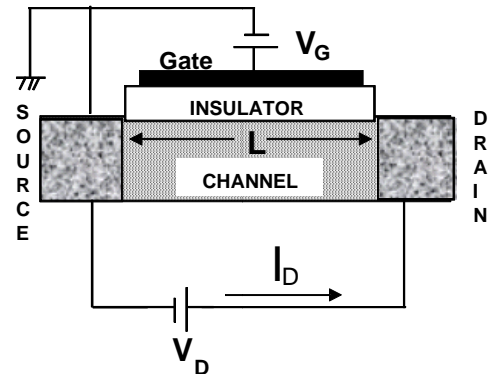
Covalent Bonding

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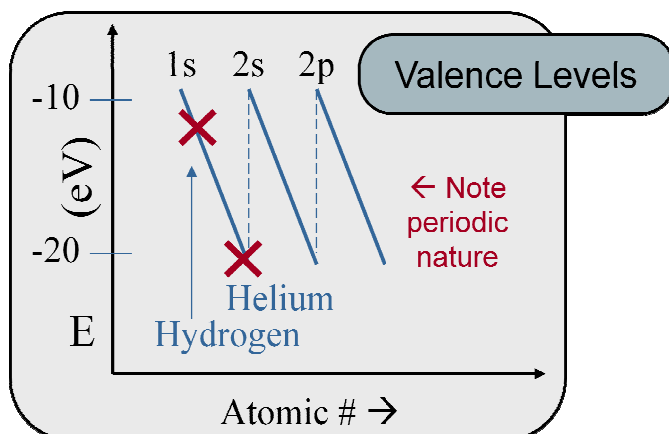
Class notes taken by: Mehdi Salmani

Schrödinger Equation

$$E\Psi = \left(-\frac{\hbar^2}{2m}\nabla^2 + U_N(\vec{r}) + U_e(\vec{r}) \right) \Psi$$



1s ¹	H							He	1s ²
	Li	Be	B	C	N	O	F	Ne	2s ² p ⁶
	Na	Mg	Al	Si	P	S	Cl	Ar	3s ² p ⁶
	K	Ca	Ga	Ge	As	Se	Br	Kr	

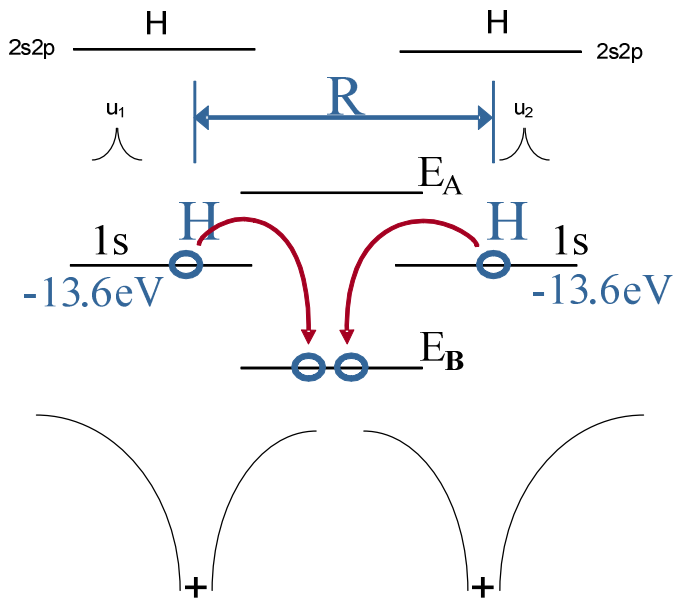


As we go down the rows and right along the columns the valence levels fill.

Note: as a level fills, going along left to right, energy levels become more negative.

It is valence electrons that really matter, for which energy levels tend to go periodically up and down.

The required energy for getting out one electron from molecule is depicted.



u_1 and u_2 are wavefunctions. And $\varphi = \varphi_1 u_1 + \varphi_2 u_2$

E_A is called **anti bonding** and E_B is called **bonding** level.

$$E\Phi = \left(-\frac{\hbar^2}{2m} \nabla^2 + U_N(\vec{r}) + U_e(\vec{r}) \right) \Phi \Rightarrow$$

$E \begin{Bmatrix} \varphi_1 \\ \varphi_2 \end{Bmatrix} = \begin{bmatrix} a & b \\ b & a \end{bmatrix} \begin{Bmatrix} \varphi_1 \\ \varphi_2 \end{Bmatrix}$ to file this matrix there are two main approaches:

1. First principle methods (Ab initio)
2. Semi-empirical methods

The eigenvalue for $\begin{bmatrix} a & b \\ b & a \end{bmatrix}$ will be $\begin{Bmatrix} a + b \\ a - b \end{Bmatrix}$.

Two types of bonding:

- Covalent bond
- Ionic bond

Usually ionic bonds are formed between atoms on opposing sides of the periodic table. Take for example Na and Cl.

Many electrical materials, such as Silicon, form through covalent bonding.

A simple example of covalent bonding: H_2 .

Covalent bonding works best with partially filled valence band. For example the group 4 elements: C, Si, Ga, etc.