Fundamentals of Nanoelectronics

ECE495 - Session 16, Sept 30, 2009

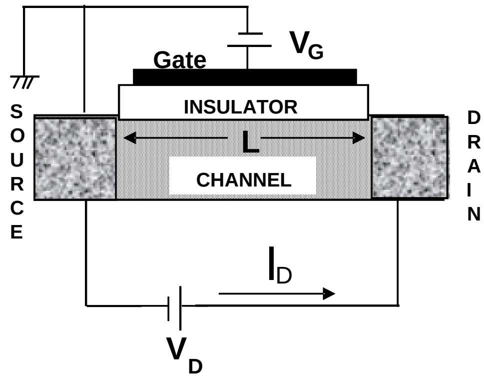
Bonding

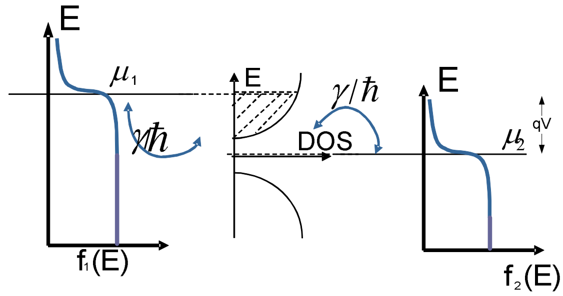
Professor Supriyo Datta

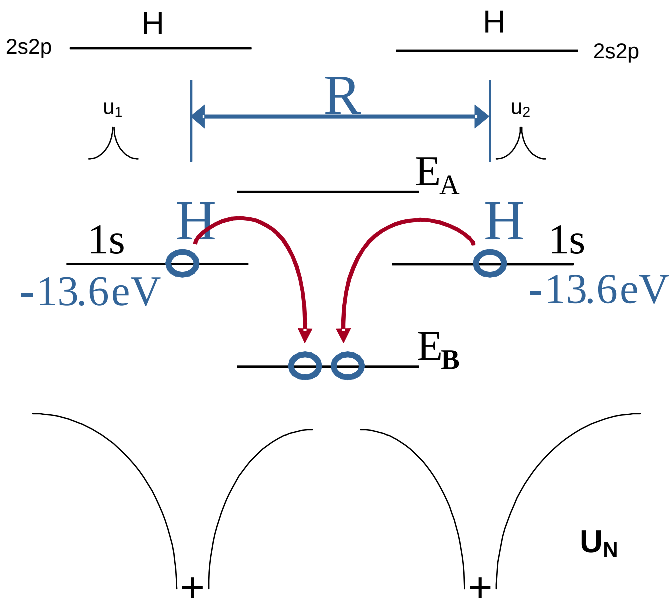
Class notes taken by: Mehdi Salmani

Schrödinger Equation

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



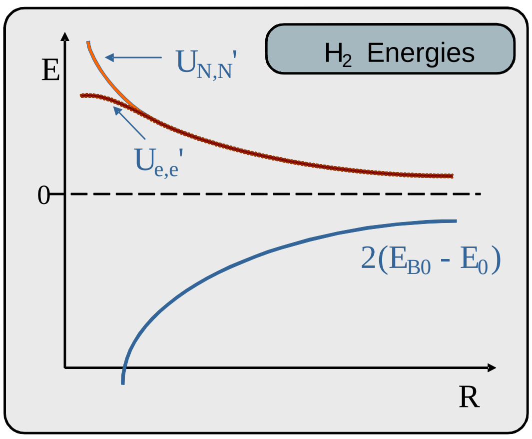




u₁ and u₂ are wavefunctions.

$$\Phi(\vec{r}) = \sum \phi_n u_n(\vec{r})$$

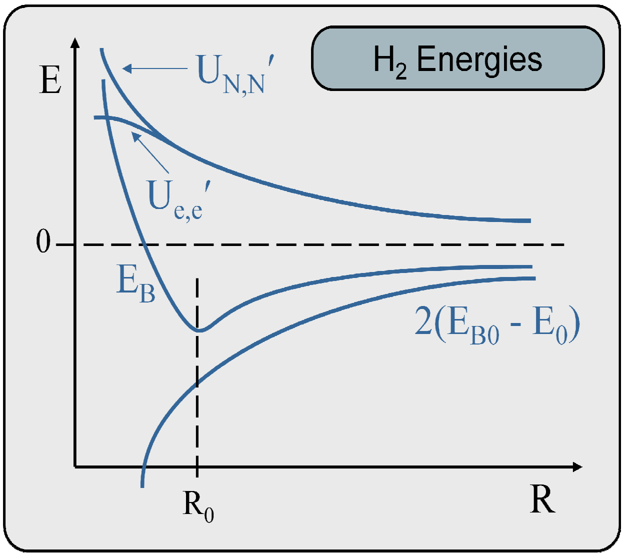
$$E\{\varphi\} = [H]\{\varphi\}$$



Since the objective is to minimize energy, a total collapse to R=0 seems to make sense. But E (blue curve) is not all energy between two nucleuses. However, we are ignoring key electron and nuclear interactions:

$E(2H) = U_{e,N} + U_{e',N'} = 2E_0$

$E(H_2) = U_{e,e'} + U_{N,N'} + U_{e,N} + U_{e,N'} + U_{e',N} + U_{e',N'}$



Just solving for 2-nuclei we get:

$\mathbf{U_{e,N} + U_{e,N}' = E_{B0}}$

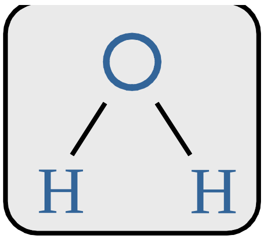
$\mathbf{U_{e}'_{,N} + U_{e}'_{,N}' = E_{B0}}$

Thus, $\mathbf{E(H_2) - E(2H) = 2(E_{B0} - E_0) + U_{e,e}' + U_{N,N}'}$

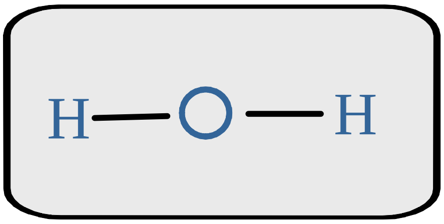
Solving for $U_{N,N}'$ is easy: $U_{N,N'} = q^2 / (4\pi\varepsilon_0 R)$

Solving for Uee is the difficult part, so we approximate: $U_{e,e'} = \dfrac{q^2}{4\pi\varepsilon_0 \sqrt{R^2 + a_0^2}}$

So, it is important to consider the full energetic…



Why the water molecule is not linear (like right hand side picture)?



However, one more point remains to be addressed, visualization of bonding as a spring mass system.

Consider the covalent bond as a spring connecting the two masses: