

Lecture 14

Last time

1) Add/subtract atomic orbital of same e^- to make molecular orbital, e.g. $1s_A + 1s_B \sim \sigma$ $0 \ 0 \rightarrow \infty$

2.) Multiply orbital of different e^- together to get Ψ (wavefunction)
e.g. H_2 has $\Psi = \sigma_+(1) \cdot \sigma_-(2)$

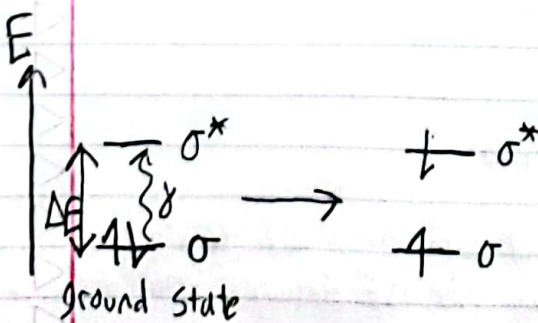
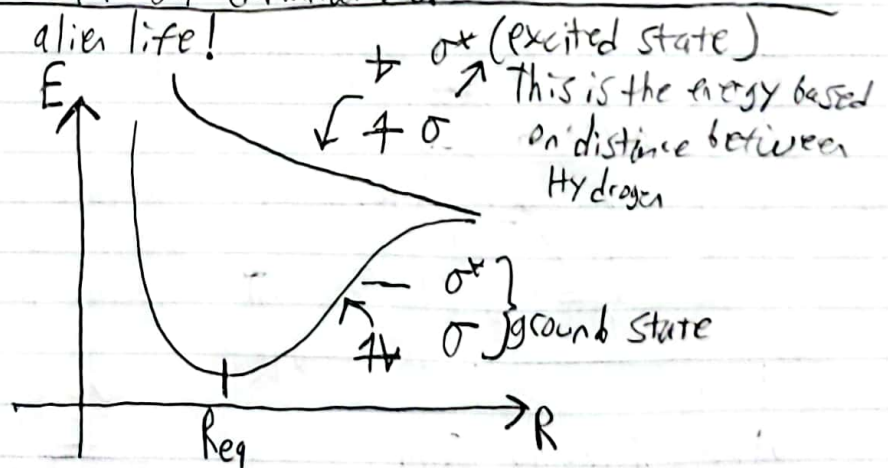
3.) make antisymmetric to satisfy Postulate 4!

e.g. H_2 has $\Psi(1,2) \sim \sigma_+(1)\sigma_-(2) - \sigma_+(2)\sigma_-(1)$

Same constant goes out front; Not important for our explanations.

Today: Spectroscopy and alien life!

e^- can be excited to higher configurations or "excited states" ex. H_2



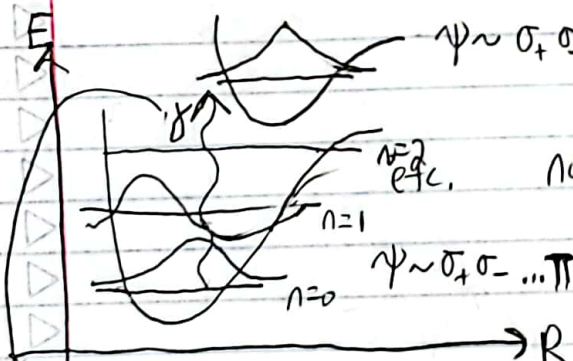
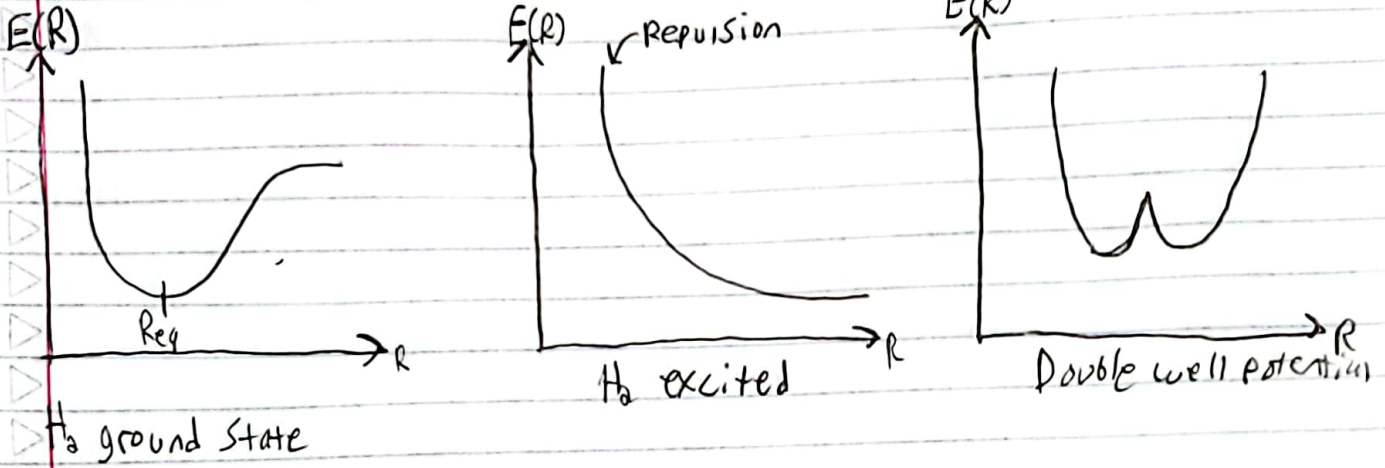
The energy of photon γ must be exactly ΔE for transition to occur

$$\Psi_{excited} \sim \sigma_+(1)\sigma_-(2) - \sigma_+(2)\sigma_-(1)$$

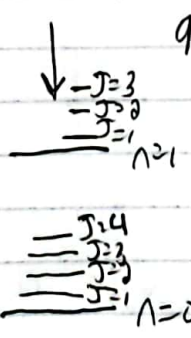
$$\Psi_{ground} \sim \sigma_+(1)\sigma_-(2) - \sigma_+(2)\sigma_-(1)$$

Spectroscopy arises from the ΔE (energy between s states)

Three Main Molecular Potential Surfaces



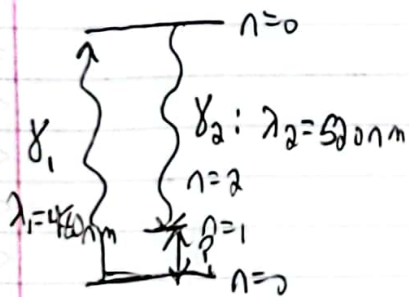
Note: We have not talked about rotational energy, but they exist for each vibrational state. Rotational energy states use quantum number "J"



Photon γ excites from lower to upper state (could be from ground or other excited vibrational states)

- Each molecule have unique frequency and can be used to detect the molecule. (the frequency comes from the ΔE between state transitions)

HW Q5.1



$$\textcircled{1} \lambda \cdot \nu = c \Rightarrow \nu = \frac{c}{\lambda}$$

$$\textcircled{2} E = h\nu \Rightarrow \Delta E = h(\nu_1 - \nu_2) = h\nu_{\text{spring}}$$

$$\textcircled{3} \nu_{\text{spring}} = \frac{\Delta E}{h} = \nu_1 - \nu_2 = \frac{c}{\lambda_1} - \frac{c}{\lambda_2}$$

Use the above strategy to find the energy between the ground state $n=1$ and $n=0$ states.