"Last" lecture for this part of the course for this section

"Journey" ———→ Expose you to Modern QM.
    – Mathematical Foundation (~1925)
        →"H- atom" Problem

(SE)

AO
pictorial view   (1e⁻ wavef.ⁿ) coordinate frame

Pauli Exclusion Principle
(antisymm. of wavef.ⁿ)

⌐→ ———→ full Wavef.ⁿ ———→

Spin Condition
"e⁻"

electron - electron repulsion

4 quantum #s.

Ignore $e^- - e^-$ repulsion: the e^- Configurations
Li

$R_{n\ell}$ Radial part $(n-\ell-1)$ nodes:

L^- Angular " $\longrightarrow$ "ℓ" nodes $\}$ $(n-1)$ Total nodes

Molecules

H_2^+

$1e^-$ case $\longrightarrow$

R

e^-

5s

4s —— 4p —— 4d —— 4f

3s —— 3p —— 3d

2s —— 2p $\ell = 2$ ...

$\ell = 1$

1s

$\ell = 0$

$\Delta \ell \neq 0$

Selection Rule $\Delta \ell = \pm 1$; $\Delta m_\ell = 0, \pm 1$
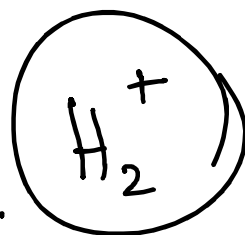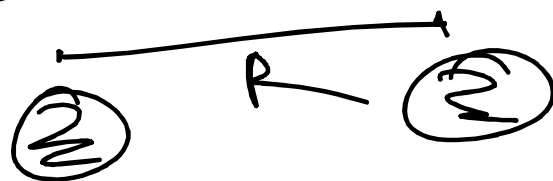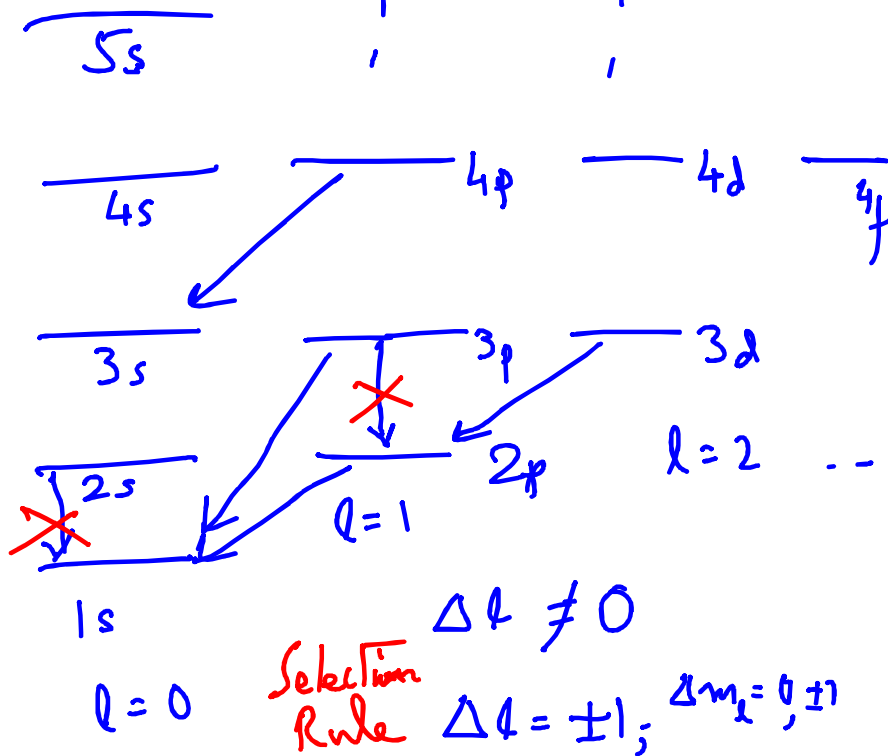
LCAO H_2^+

$H\Psi = E(R)\Psi$

diff. "R" values.

Bonding
Antibonding
Nonbonding

O_2 configuration

Born - Oppenheimer Approx.

Franck - Condon "Principle"

"Electronic Spectroscopy"

Bond Order $\rightarrow \frac{1}{2}(N_B - N_A)$

S_1

R

E

$V=2$
$V=1$
$V=0$

S_0
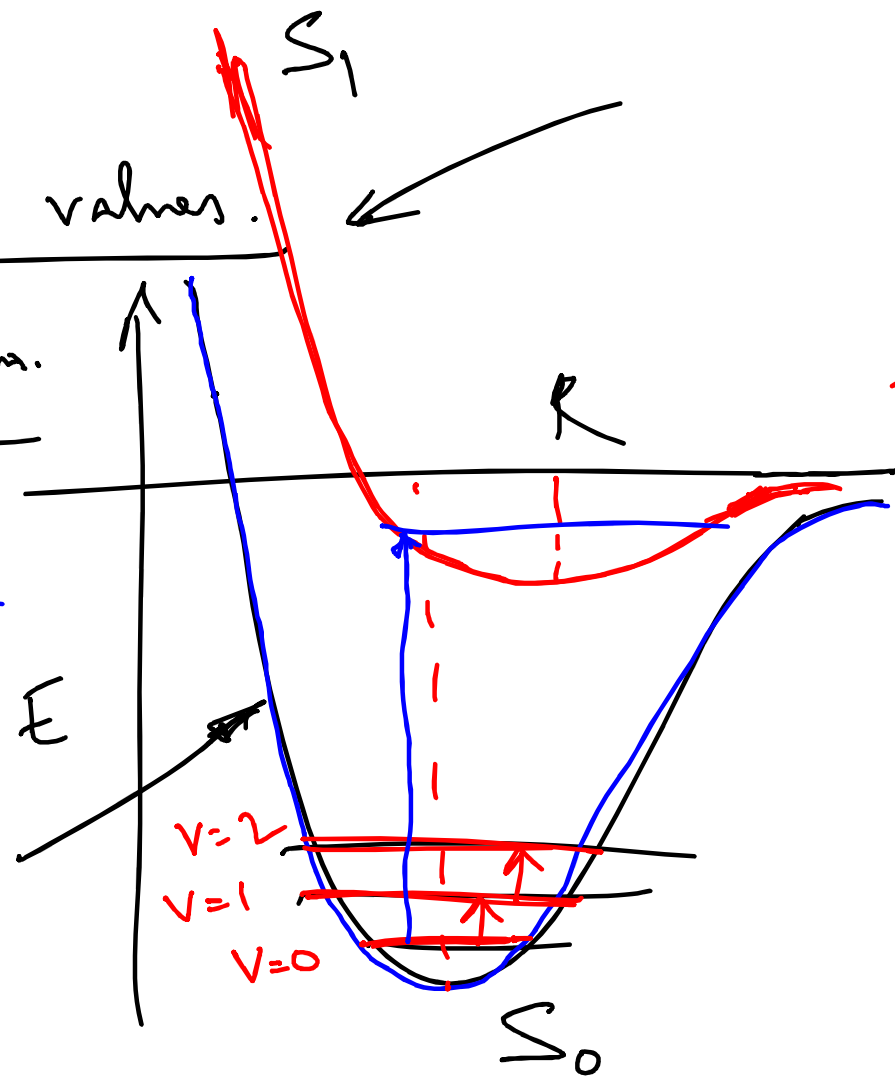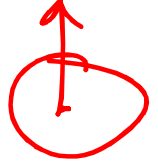
Rotational Spectroscopy

Applied field & Molecule $\longrightarrow$

$\boxed{1^{st} \text{ eg.}}$

$\underline{\text{Dipole approximation}}$

$\overline{\text{Charge Dipole formation}}$

$"E" \longrightarrow$

non-symmetry