

ATOMS

$$H_{\text{eff}} \Psi = E \Psi$$

Ψ IS A GUESS AND A
LINEAR COMBINATION OF
SLATER ORBITALS

$$S_{nlm}(r, \theta, \varphi) = N_{nl} r^{n-1} e^{-\zeta r} Y_l^m(\theta, \varphi)$$

$$N_{nl} = \text{CONSTANT}$$

PARAMETER ARE OPTIMIZED TO GET
THE BEST POSSIBLE DESCRIPTION OF
THE ATOMIC ENERGY LEVELS

ADD SPIN AND FILL ENERGY LEVELS

MOLECULES

BORN-OPPENHEIMER APPROX (1927)

Freeze the nuclei AND SOLVE FOR
electrons! THEREFORE THE
ENERGY DEPENDS ON NUCLEAR
COORDINATES.

— ONLY ORBITAL WITH SIMILAR ENERGY MIX.

— ONLY ORBITAL WITH SIGNIFICANT OVERLAP MIX.

Molecules $H_2(g)$

① 1s
2s
2p

1s ②
2s
2p

