

HF-SCF-AO

Hartree-Fock - Self Consistent Field Atomic Orbitals
Numerical Solution of Schrodinger Equation
for many electron atom

$$-\frac{\hbar^2}{2m_e} \nabla^2 \psi_{3s} - \left(\frac{Ze^2}{4\pi\epsilon_0 r} \right) \psi_{3s} + V_{ee} \psi_{3s} = E \psi_{3s}$$

for 3s orbital in Na $1s^2 2s^2 2p^6 3s^1$

Assume $1s^2 2s^2 2p^6$ use for V_{ee}

Find new and improved 3s

allow change
in just
1 orbital

Use $1s^2 2s^2 2p^5$ "3s" calculate 2p then 2s then 1s
and repeat starting with 3s again

Continue process until new orbitals are
not different from last cycle
orbitals are self-consistent