

Calculating Hartree-Fock SCF potential energy surfaces

- 1) Pick nuclear coordinates \vec{R}_m of the molecule(s)
- 2) Guess MO or VB basis functions with coefficients c_m
- 3) Calculate N Fock operators
- 4) Solve N 1-electron Schrödinger equations
- 5) Go back to 3 and iterate until coefficients c_m converge to the lowest variational energy
- 6) You now have $E_{HF}(\vec{R}_m)$; go back to 1) and pick a different set \vec{R}_m
- 7) Plot the whole potential energy surface $E(\vec{R}_m)$

SN2 reaction:
hydroxide + methyl iodide

