

$$\Phi(1, 2) = 1/\sqrt{2} [\varphi_1(1)\varphi_2(2) - \varphi_1(2)\varphi_2(1)]$$

$$\hat{H} = \hat{h}(1) + \hat{h}(2) + \frac{1}{r_{12}} \quad E = \langle \Phi(1, 2) | \hat{H} | \Phi(1, 2) \rangle$$

$$\begin{aligned} E &= \frac{1}{2} \left\langle \varphi_1(1)\varphi_2(2) - \varphi_1(2)\varphi_2(1) \left| \hat{h}(1) + \hat{h}(2) + \frac{1}{r_{12}} \right| \varphi_1(1)\varphi_2(2) - \varphi_1(2)\varphi_2(1) \right\rangle = \\ &= \frac{1}{2} \left\langle \varphi_1(1)\varphi_2(2) - \varphi_1(2)\varphi_2(1) \left| \hat{h}(1) \right| \varphi_1(1)\varphi_2(2) - \varphi_1(2)\varphi_2(1) \right\rangle + \\ &+ \frac{1}{2} \left\langle \varphi_1(1)\varphi_2(2) - \varphi_1(2)\varphi_2(1) \left| \hat{h}(2) \right| \varphi_1(1)\varphi_2(2) - \varphi_1(2)\varphi_2(1) \right\rangle + \\ &+ \frac{1}{2} \left\langle \varphi_1(1)\varphi_2(2) - \varphi_1(2)\varphi_2(1) \left| \frac{1}{r_{12}} \right| \varphi_1(1)\varphi_2(2) - \varphi_1(2)\varphi_2(1) \right\rangle = \end{aligned}$$

$$\begin{aligned} &= \frac{1}{2} \langle \varphi_1(1)\varphi_2(2) | \hat{h}(1) | \varphi_1(1)\varphi_2(2) \rangle + \frac{1}{2} \langle \varphi_2(1)\varphi_1(2) | \hat{h}(1) | \varphi_2(1)\varphi_1(2) \rangle - \\ &- \frac{1}{2} \langle \varphi_1(1)\varphi_2(2) | \hat{h}(1) | \varphi_2(1)\varphi_1(2) \rangle - \frac{1}{2} \langle \varphi_2(1)\varphi_1(2) | \hat{h}(1) | \varphi_1(1)\varphi_2(2) \rangle + \end{aligned}$$

$$\begin{aligned} &+ \frac{1}{2} \langle \varphi_1(1)\varphi_2(2) | \hat{h}(2) | \varphi_1(1)\varphi_2(2) \rangle + \frac{1}{2} \langle \varphi_2(1)\varphi_1(2) | \hat{h}(2) | \varphi_2(1)\varphi_1(2) \rangle - \\ &- \frac{1}{2} \langle \varphi_1(1)\varphi_2(2) | \hat{h}(2) | \varphi_2(1)\varphi_1(2) \rangle - \frac{1}{2} \langle \varphi_2(1)\varphi_1(2) | \hat{h}(2) | \varphi_1(1)\varphi_2(2) \rangle + \end{aligned}$$

$$\begin{aligned} &+ \frac{1}{2} \left\langle \varphi_1(1)\varphi_2(2) \left| \frac{1}{r_{12}} \right| \varphi_1(1)\varphi_2(2) \right\rangle + \frac{1}{2} \left\langle \varphi_2(1)\varphi_1(2) \left| \frac{1}{r_{12}} \right| \varphi_2(1)\varphi_1(2) \right\rangle - \\ &- \frac{1}{2} \left\langle \varphi_1(1)\varphi_2(2) \left| \frac{1}{r_{12}} \right| \varphi_2(1)\varphi_1(2) \right\rangle - \frac{1}{2} \left\langle \varphi_2(1)\varphi_1(2) \left| \frac{1}{r_{12}} \right| \varphi_1(1)\varphi_2(2) \right\rangle = \end{aligned}$$

$$\begin{aligned} &= \frac{1}{2} \langle \varphi_1(1) | \hat{h}(1) | \varphi_1(1) \rangle + \frac{1}{2} \langle \varphi_2(1) | \hat{h}(1) | \varphi_2(1) \rangle + \\ &+ \frac{1}{2} \langle \varphi_1(2) | \hat{h}(2) | \varphi_1(2) \rangle + \frac{1}{2} \langle \varphi_2(2) | \hat{h}(2) | \varphi_2(2) \rangle + \end{aligned}$$

$$\begin{aligned} &+ \frac{1}{2} \left\langle \varphi_1(1)\varphi_2(2) \left| \frac{1}{r_{12}} \right| \varphi_1(1)\varphi_2(2) \right\rangle + \frac{1}{2} \left\langle \varphi_2(1)\varphi_1(2) \left| \frac{1}{r_{12}} \right| \varphi_2(1)\varphi_1(2) \right\rangle - \\ &- \frac{1}{2} \left\langle \varphi_1(1)\varphi_2(2) \left| \frac{1}{r_{12}} \right| \varphi_2(1)\varphi_1(2) \right\rangle - \frac{1}{2} \left\langle \varphi_2(1)\varphi_1(2) \left| \frac{1}{r_{12}} \right| \varphi_1(1)\varphi_2(2) \right\rangle = \end{aligned}$$

$$= \langle \mathbf{1} | \hat{h} | \mathbf{1} \rangle + \langle \mathbf{2} | \hat{h} | \mathbf{2} \rangle + \frac{1}{2} \left\langle \mathbf{12} \left| \frac{1}{r_{12}} \right| \mathbf{12} \right\rangle + \frac{1}{2} \left\langle \mathbf{21} \left| \frac{1}{r_{12}} \right| \mathbf{21} \right\rangle - \frac{1}{2} \left\langle \mathbf{12} \left| \frac{1}{r_{12}} \right| \mathbf{21} \right\rangle - \frac{1}{2} \left\langle \mathbf{21} \left| \frac{1}{r_{12}} \right| \mathbf{12} \right\rangle$$

$$E = \varepsilon_1 + \varepsilon_2 + J - K = \sum_{i=1}^2 \varepsilon_i + \frac{1}{2} \sum_{i=1}^2 \sum_{j=1}^2 (J_{ij} - K_{ij}), \quad J_{ii} = K_{ii} = 0$$

$$F = E - \sum_{i=1}^2 \sum_{j=1}^2 (\varepsilon_{ij} \langle \varphi_i | \varphi_j \rangle - \delta_{ij})$$

$$\begin{aligned} \delta F = & \langle \delta \mathbf{1} | \hat{h} | \mathbf{1} \rangle + \langle \delta \mathbf{2} | \hat{h} | \mathbf{2} \rangle + \\ & + \frac{1}{2} \left\langle \delta \mathbf{1} \mathbf{2} \left| \frac{1}{r_{12}} \right| \mathbf{1} \mathbf{2} \right\rangle + \frac{1}{2} \left\langle \mathbf{1} \delta \mathbf{2} \left| \frac{1}{r_{12}} \right| \mathbf{1} \mathbf{2} \right\rangle + \frac{1}{2} \left\langle \delta \mathbf{2} \mathbf{1} \left| \frac{1}{r_{12}} \right| \mathbf{2} \mathbf{1} \right\rangle + \frac{1}{2} \left\langle \mathbf{2} \delta \mathbf{1} \left| \frac{1}{r_{12}} \right| \mathbf{2} \mathbf{1} \right\rangle - \\ & - \frac{1}{2} \left\langle \delta \mathbf{1} \mathbf{2} \left| \frac{1}{r_{12}} \right| \mathbf{2} \mathbf{1} \right\rangle - \frac{1}{2} \left\langle \delta \mathbf{2} \mathbf{1} \left| \frac{1}{r_{12}} \right| \mathbf{1} \mathbf{2} \right\rangle - \frac{1}{2} \left\langle \mathbf{1} \delta \mathbf{2} \left| \frac{1}{r_{12}} \right| \mathbf{2} \mathbf{1} \right\rangle - \frac{1}{2} \left\langle \mathbf{2} \delta \mathbf{1} \left| \frac{1}{r_{12}} \right| \mathbf{1} \mathbf{2} \right\rangle - \\ & - \varepsilon_{11} \langle \delta \mathbf{1} | \mathbf{1} \rangle - \varepsilon_{12} \langle \delta \mathbf{1} | \mathbf{2} \rangle - \varepsilon_{21} \langle \delta \mathbf{2} | \mathbf{1} \rangle - \varepsilon_{22} \langle \delta \mathbf{2} | \mathbf{2} \rangle + \\ & + \text{c. c.} = 0 \end{aligned}$$

$$\left(\hat{h} + \frac{1}{2} \left\langle \cdot \mathbf{2} \left| \frac{1}{r_{12}} \right| \cdot \mathbf{2} \right\rangle + \frac{1}{2} \left\langle \mathbf{2} \cdot \left| \frac{1}{r_{12}} \right| \mathbf{2} \cdot \right\rangle - \frac{1}{2} \left\langle \cdot \mathbf{2} \left| \frac{1}{r_{12}} \right| \mathbf{2} \cdot \right\rangle - \frac{1}{2} \left\langle \mathbf{2} \cdot \left| \frac{1}{r_{12}} \right| \cdot \mathbf{2} \right\rangle \right) | \mathbf{1} \rangle = \varepsilon_{11} | \mathbf{1} \rangle + \varepsilon_{12} | \mathbf{2} \rangle$$

$$\left(\hat{h} + \frac{1}{2} \left\langle \cdot \mathbf{1} \left| \frac{1}{r_{12}} \right| \cdot \mathbf{1} \right\rangle + \frac{1}{2} \left\langle \mathbf{1} \cdot \left| \frac{1}{r_{12}} \right| \mathbf{1} \cdot \right\rangle - \frac{1}{2} \left\langle \cdot \mathbf{1} \left| \frac{1}{r_{12}} \right| \mathbf{1} \cdot \right\rangle - \frac{1}{2} \left\langle \mathbf{1} \cdot \left| \frac{1}{r_{12}} \right| \cdot \mathbf{1} \right\rangle \right) | \mathbf{2} \rangle = \varepsilon_{21} | \mathbf{1} \rangle + \varepsilon_{22} | \mathbf{2} \rangle$$

Canonical HF-Equations

$$\left(\hat{h} + \left\langle \cdot \mathbf{2} \left| \frac{1}{r_{12}} \right| \cdot \mathbf{2} \right\rangle - \left\langle \cdot \mathbf{2} \left| \frac{1}{r_{12}} \right| \mathbf{2} \cdot \right\rangle \right) | \mathbf{1} \rangle = \varepsilon_{11} | \mathbf{1} \rangle$$

$$\left(\hat{h} + \left\langle \cdot \mathbf{1} \left| \frac{1}{r_{12}} \right| \cdot \mathbf{1} \right\rangle - \left\langle \cdot \mathbf{1} \left| \frac{1}{r_{12}} \right| \mathbf{1} \cdot \right\rangle \right) | \mathbf{2} \rangle = \varepsilon_{22} | \mathbf{2} \rangle$$

Columb operator

$$\hat{J}_{\mathbf{2}} | \mathbf{1} \rangle = \left\langle \cdot \mathbf{2} \left| \frac{1}{r_{12}} \right| \cdot \mathbf{2} \right\rangle | \mathbf{1} \rangle = \int \frac{\cdot \varphi_{\mathbf{2}}(2) \cdot \varphi_{\mathbf{2}}(2)}{r_{12}} d(2) \cdot \varphi_{\mathbf{1}}(1) = \int \frac{\cdot \varphi_{\mathbf{2}}(2) \varphi_{\mathbf{1}}(1) \varphi_{\mathbf{2}}(2)}{r_{12}} d(2)$$

Columb integral

$$\langle \mathbf{1} | \hat{J}_{\mathbf{2}} | \mathbf{1} \rangle = \langle \mathbf{1} | \left\langle \cdot \mathbf{2} \left| \frac{1}{r_{12}} \right| \cdot \mathbf{2} \right\rangle | \mathbf{1} \rangle = \iint \frac{\varphi_{\mathbf{1}}(1) \varphi_{\mathbf{2}}(2) \varphi_{\mathbf{1}}(1) \varphi_{\mathbf{2}}(2)}{r_{12}} d(2) d(1)$$

Exchange operator

$$\hat{K}_{\mathbf{2}} | \mathbf{1} \rangle = \left\langle \cdot \mathbf{2} \left| \frac{1}{r_{12}} \right| \mathbf{2} \cdot \right\rangle | \mathbf{1} \rangle = \int \frac{\cdot \varphi_{\mathbf{2}}(2) \varphi_{\mathbf{2}}(1) \cdot}{r_{12}} d(2) \cdot \varphi_{\mathbf{1}}(1) = \int \frac{\cdot \varphi_{\mathbf{2}}(2) \varphi_{\mathbf{2}}(1) \varphi_{\mathbf{1}}(2)}{r_{12}} d(2)$$

Exchange integral

$$\langle \mathbf{1} | \hat{K}_{\mathbf{2}} | \mathbf{1} \rangle = \langle \mathbf{1} | \left\langle \cdot \mathbf{2} \left| \frac{1}{r_{12}} \right| \mathbf{2} \cdot \right\rangle | \mathbf{1} \rangle = \iint \frac{\varphi_{\mathbf{1}}(1) \varphi_{\mathbf{2}}(2) \varphi_{\mathbf{2}}(1) \varphi_{\mathbf{1}}(2)}{r_{12}} d(2) d(1)$$