

$$\mathbf{S}\mathbf{L}_S = \mathbf{L}_S\Lambda_S$$

$$\mathbf{S}^{-1/2} \equiv \mathbf{L}_S\Lambda^{-1/2}\tilde{\mathbf{L}}_S$$

$$\mathbf{F}_0' \equiv \tilde{\mathbf{S}}^{-1/2} \mathbf{H}^{\text{core}} \mathbf{S}^{-1/2}$$

$$\mathbf{F}_0'\mathbf{C}_0'=\mathbf{C}_0'\epsilon_0$$

$$\mathbf{C}_0=\mathbf{S}^{-1/2}\mathbf{C}_0'$$

$$D_{\mu\nu}^0=\sum_m^{\text{occ}}(\mathbf{C}_0)^m_{\mu}(\mathbf{C}_0)^m_{\nu}$$

$$E_{\text{elec}}^0=\sum_{\mu\nu}^{\text{AO}}D_{\mu\nu}^0(H_{\mu\nu}^{\text{core}}+F_{\mu\nu})$$

$$=\text{tr}(\mathbf{D}(\mathbf{H}^{\text{core}}+\mathbf{F}))$$

$$E_{\text{total}}^0=E_{\text{elec}}^0+E_{\text{nuc}}$$

$$\mathbf{F}'\equiv\tilde{\mathbf{S}}^{-1/2}\mathbf{F}^{\text{core}}\mathbf{S}^{-1/2}$$

$$\mathbf{F}'\mathbf{C}'=\mathbf{C}'\epsilon$$

$$\mathbf{C}=\mathbf{S}^{-1/2}\mathbf{C}'$$

$$E_{\text{elec}}^i=\sum_{\mu\nu}^{\text{AO}}D_{\mu\nu}(H_{\mu\nu}^{\text{core}}+F_{\mu\nu})$$

$$E_{\text{total}}^i=E_{\text{elec}}^i+E_{\text{nuc}}$$

$$\Delta E=E_{\text{elec}}^i-E_{\text{elec}}^{i-1}<\delta_1$$

$$\text{rms}_D=\left[\sum_{\mu\nu}(D_{\mu\nu}^i-D_{\mu\nu}^{i-1})^2\right]^{1/2}<\delta_2$$

$$\hat{F}\chi_i=\epsilon_i\chi_i$$

$$(\mathbf{F})_{ij}\equiv\epsilon_i\delta_{ij}=\langle\chi_j|\hat{F}|\chi_i\rangle$$

$$(\mathbf{F})_{ij}=\sum_{\mu\nu}C_{\mu}^jC_{\nu}^i\,\langle\phi_{\mu}|\hat{F}|\phi_{\nu}\rangle=\sum_{\mu\nu}C_{\mu}^jC_{\nu}^iF_{\mu\nu}$$

$$\langle \vec{\mu} \rangle = 2 \sum_{\mu\nu} D_{\mu\nu} \, \langle \phi_{\mu} | \vec{\mu} | \phi_{\nu} \rangle$$

$$q_A=Z_A-2\sum_{\mu\in A}(\mathbf{D}\mathbf{S})_{\mu\mu}$$