



PSI4

AB INITIO QUANTUM CHEMISTRY

$$\left[\sum_{\alpha} \frac{\partial^2}{\partial x_{\alpha}^2} + \sum_{\alpha} \frac{\partial^2}{\partial y_{\alpha}^2} + \sum_{\alpha} \frac{\partial^2}{\partial z_{\alpha}^2} \right] \Psi(r; R) = E_{\text{el}} \Psi(r; R) \quad E_{\text{Nuc-Rep}} = \sum_{\alpha\beta} \left(E_{\text{rep}}^{(\alpha\beta)} + E_{\text{rep}}^{(\beta\alpha)} \right) \quad E_{\text{CC}} = \sum_{\alpha} f_{\alpha} c_{\alpha}^{\dagger} + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle ij || ab \rangle c_{\alpha}^{\dagger} c_{\beta}^{\dagger} + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle ij || ab \rangle c_{\alpha}^{\dagger} c_{\beta}^{\dagger} \quad |\Psi\rangle = c_0 |\Phi_0\rangle + \sum_{\alpha} c_{\alpha} c_{\alpha}^{\dagger} |\Phi_{\alpha}^{\alpha}\rangle + \sum_{\alpha} \sum_{\beta} c_{\alpha} c_{\beta}^{\dagger} |\Phi_{\alpha\beta}^{\alpha\beta}\rangle + \sum_{\alpha\beta} \sum_{\gamma\delta} c_{\alpha}^{\dagger} c_{\beta}^{\dagger} |\Phi_{\alpha\beta}^{\alpha\beta}\rangle + \dots \quad \text{FC} = \text{SCF} \quad E_{\text{el}} = \frac{1}{2} \sum_{\alpha\beta} c_{\alpha}^{\dagger} c_{\beta}^{\dagger} D_{\alpha\beta}^{\text{el}} \left[c_{\alpha}^{\dagger} c_{\beta}^{\dagger} + c_{\alpha}^{\dagger} c_{\beta}^{\dagger} \right]$$

$$\text{FC} = \text{SCF} \quad |\Psi\rangle = c_0 |\Phi_0\rangle + \sum_{\alpha} c_{\alpha} c_{\alpha}^{\dagger} |\Phi_{\alpha}^{\alpha}\rangle + \sum_{\alpha} \sum_{\beta} c_{\alpha} c_{\beta}^{\dagger} |\Phi_{\alpha\beta}^{\alpha\beta}\rangle + \sum_{\alpha\beta} \sum_{\gamma\delta} c_{\alpha}^{\dagger} c_{\beta}^{\dagger} |\Phi_{\alpha\beta}^{\alpha\beta}\rangle + \dots \quad E_{\text{Nuc-Rep}} = \sum_{\alpha\beta} \left(E_{\text{rep}}^{(\alpha\beta)} + E_{\text{rep}}^{(\beta\alpha)} \right) \quad E_{\text{Nuc-Rep}} = \sum_{\alpha\beta} \sum_{\gamma\delta} (ia || jb) \left[2(ia || jb) - (ib || ja) \right] \left[c_{\alpha}^{\dagger} c_{\beta}^{\dagger} - c_{\alpha}^{\dagger} c_{\beta}^{\dagger} \right] \quad \langle \mu\nu || \lambda\sigma \rangle = \int \phi_{\mu}(r_1) \phi_{\nu}(r_1) c_{\mu}^{\dagger} c_{\nu}^{\dagger} \phi_{\lambda}(r_2) \phi_{\sigma}(r_2) dr_1 dr_2 \quad E_{\text{CC}} = \sum_{\alpha} f_{\alpha} c_{\alpha}^{\dagger} + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle ij || ab \rangle c_{\alpha}^{\dagger} c_{\beta}^{\dagger} + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle ij || ab \rangle c_{\alpha}^{\dagger} c_{\beta}^{\dagger} \quad \left[+ \sum_{\alpha} V_{\alpha}^{\dagger} - \sum_{\alpha} \frac{1}{r_{\alpha}} + \sum_{\alpha} \frac{1}{r_{\alpha}} + \sum_{\alpha} \frac{1}{r_{\alpha}} \right] \Psi(r; R) = E_{\text{el}} \Psi(r; R)$$