



PSI4

OPEN-SOURCE QUANTUM CHEMISTRY

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

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