



PSI4

OPEN-SOURCE QUANTUM CHEMISTRY

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

$$\text{FC} = \text{SCF} \quad |\Psi\rangle = c_0 |\Phi_0\rangle + \sum_{\alpha} c'_{\alpha} |\Phi'_{\alpha}\rangle + \sum_{\alpha} \sum_{\alpha'} c''_{\alpha} |\Phi''_{\alpha}\rangle + \sum_{\alpha} \sum_{\alpha'} c'''_{\alpha} |\Phi'''_{\alpha}\rangle + \dots \quad E_{\text{Nuc-Rep}} = \sum_{\alpha\beta} \left(E_{\text{rep}}^{(\alpha\beta)} + E_{\text{rep}}^{(\beta\alpha)} \right) \quad E_{\text{Nuc-Rep}} = \sum_{\alpha\beta} \sum_{\alpha'} \langle \alpha\alpha' || \beta\beta' \rangle \left[2 \langle \alpha\alpha' || \beta\beta' \rangle - \langle \alpha\alpha' || \beta\beta' \rangle \right] \left[c_{\alpha} + c_{\alpha'} - c_{\beta} - c_{\beta'} \right] \quad \langle \mu\nu || \lambda\sigma \rangle = \int \phi_{\mu}(r_1) \phi_{\nu}(r_1) c'_{\mu} c'_{\nu} \phi_{\lambda}(r_2) \phi_{\sigma}(r_2) dr_1 dr_2 \quad E_{\text{CC}} = \sum_{\alpha} f_{\alpha} c'_{\alpha} + \frac{1}{2} \sum_{\alpha\beta} \langle ij || ab \rangle c'_{\alpha} c'_{\beta} + \frac{1}{2} \sum_{\alpha\beta} \langle ij || ab \rangle c'_{\alpha} c'_{\beta} \quad \left[+ \sum_{\alpha} V'_{\alpha} - \sum_{\alpha} \frac{f_{\alpha}}{c_{\alpha}} + \sum_{\alpha} \frac{f_{\alpha}}{c_{\alpha}} + \sum_{\alpha} \frac{f_{\alpha}}{c_{\alpha}} \right] \Psi(r; R) = E_{\text{el}} \Psi(r; R)$$