



$$\left[-\sum_{i=1}^N \sum_{A=1}^M \frac{Z_A}{r_{iA}} + \sum_{i=1}^N \sum_{j>i}^N \frac{1}{r_{ij}} + \sum_{A=1}^M \sum_{B>A}^M \frac{Z_A Z_B}{R_{AB}} \right] \Psi = E \Psi$$

$$\int \rho(\mathbf{r}_1) d\mathbf{r}_1 + T[\rho] - \int \frac{\rho(\mathbf{r}_1)\rho(\mathbf{r}_2)}{r_{12}} d\mathbf{r}_1 d\mathbf{r}_2 + E_{XC}[\rho]$$

$$+ \frac{1}{2} \sum_{AB} V_{AB}^{\text{rep}} + \frac{1}{2} \sum_{AB} \Delta q_A \Delta q_B \gamma_{AB} + \frac{1}{3} \sum_{AB} \Delta q_A^2 \Delta q_B \Gamma_{AB}$$

$\chi_\mu^B \rangle$

$$+ \sum_{N \in A} V^{\text{NR}} + \sum_{N \in A} V^+ | \chi_\nu^B \rangle \quad (A = B)$$

$$+ \sum_{N \in A, B} V^{\text{NR}} + \sum_{N \in A, B} V^+ | \chi_\nu^B \rangle \quad (A \neq B, R_{AB} \leq \tau)$$

$$(A \neq B, R_{AB} > \tau)$$



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rhoa = rhoa + vmo(imo, 1) * vmo(imo, 1)
rhoa(1) = rhoa(1) + vmo(imo, 2) * vmo(imo, 2)
rhoa(2) = rhoa(2) + vmo(imo, 3) * vmo(imo, 3)
rhoa(3) = rhoa(3) + vmo(imo, 4) * vmo(imo, 4)
enddo

if((rhoa*two) < rcutoff) cycle
rhoa(1) = rhoa(1) * two
rhoa(2) = rhoa(2) * two
rhoa(3) = rhoa(3) * two

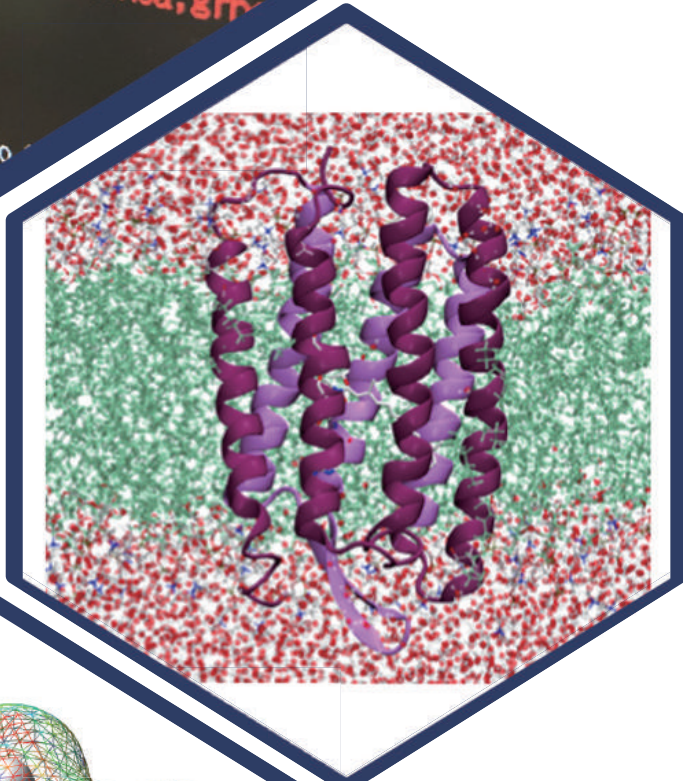
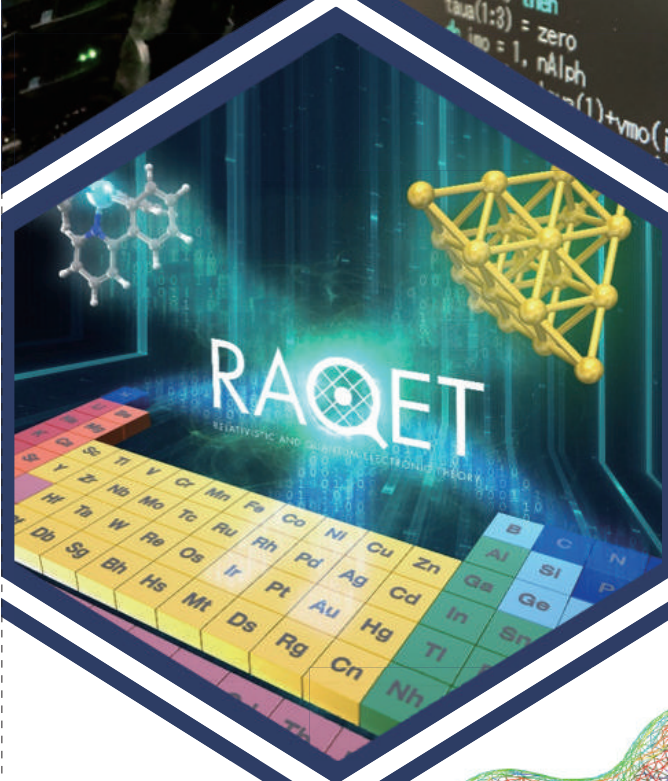
call calcexcor(excora, excora, rhoa, rhoa, grho)

if(metaagg4) then
taua(1:3) = zero
imo = 1, nAlph
rhoa(1) + vmo(imo

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$$\langle \mu_j^\alpha | a^\alpha b^\alpha \rangle (2\tilde{t}_{ij,ab}^\alpha - \tilde{t}_{ij,ba}^\alpha)$$

$$+ \frac{1}{2} \sum_I^{\text{nuc}} \sum_J^{\text{nuc}} \langle \phi_I \phi_J | \phi_I \phi_J \rangle$$



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