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

$$\int \frac{\rho(\mathbf{r}_1)}{\mathbf{r}_{1A}} d\mathbf{r}_1 + T[\rho] - \int \frac{\rho(\mathbf{r}_1)\rho(\mathbf{r}_1)}{\mathbf{r}_{12}} d\mathbf{r}_1 \mathbf{r}_2 + E_{XC}[\rho]$$

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

$$\left| \chi_\mu^B \right\rangle$$

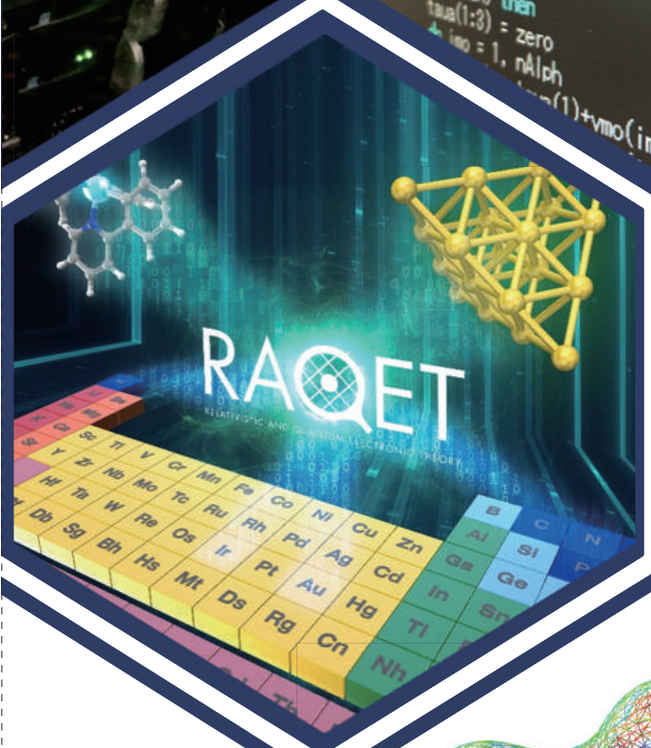
$$+ \sum V^{\mathrm{NR}} + \sum_{N \notin A} V^{+} \left| \chi_\nu^B \right\rangle \qquad (A = B)$$

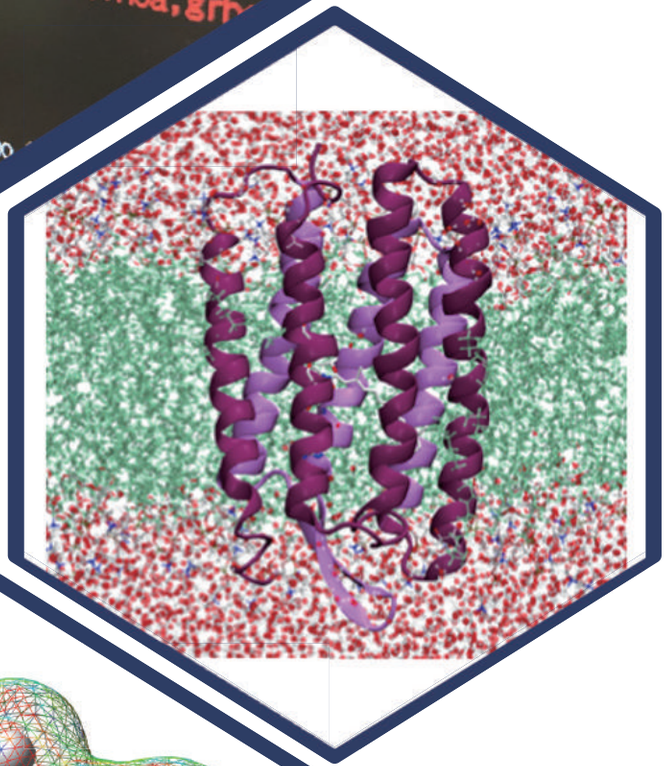
$$V^{\mathrm{NR}} + \sum_{N \notin A,B} V^{+} \left| \chi_\nu^B \right\rangle \qquad (A \neq B, R_{AB} \leq \tau)$$

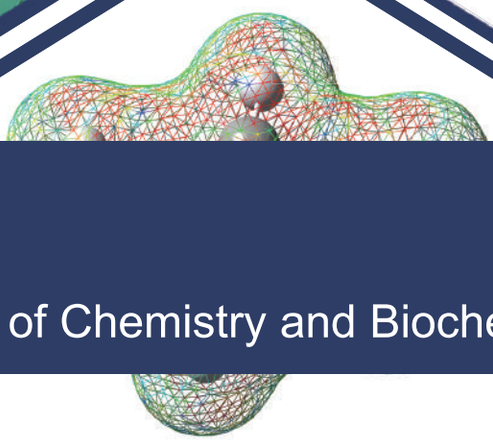
$$(A \neq B, R_{AB} > \tau)$$

$$\left\langle \mu j^\alpha \left| a^\alpha b^\alpha \right\rangle \left(2\tilde{t}_{ij,ab}^{\alpha} - \tilde{t}_{ij,ba}^{\alpha} \right) \right.$$

$$\left. \right\rangle + \frac{1}{2}\sum_{I}^{\mathrm{nuc}}\sum_{J}^{\mathrm{nuc}} \left\langle \phi_I \phi_J \left| \phi_I \phi_J \right. \right\rangle$$







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