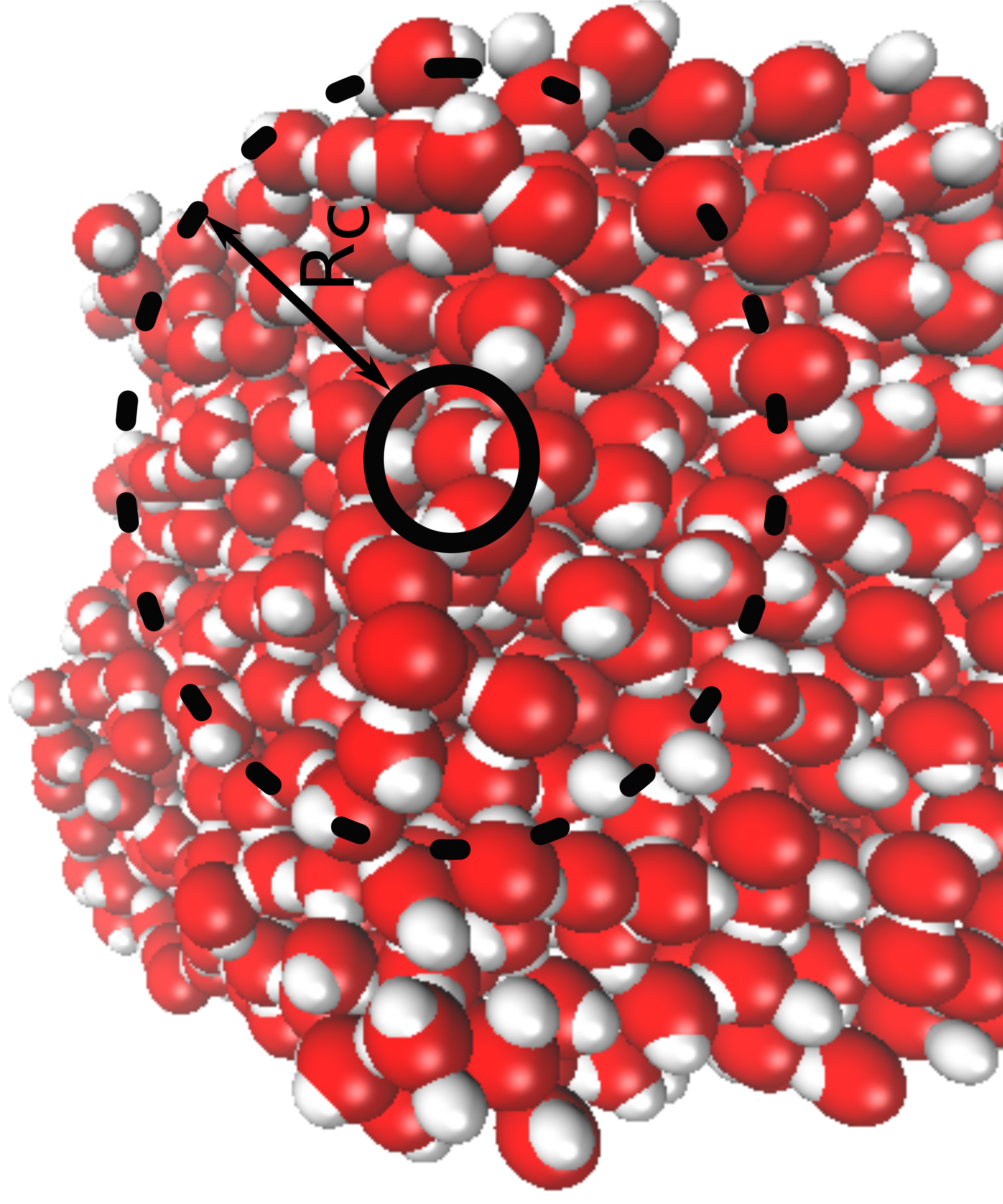
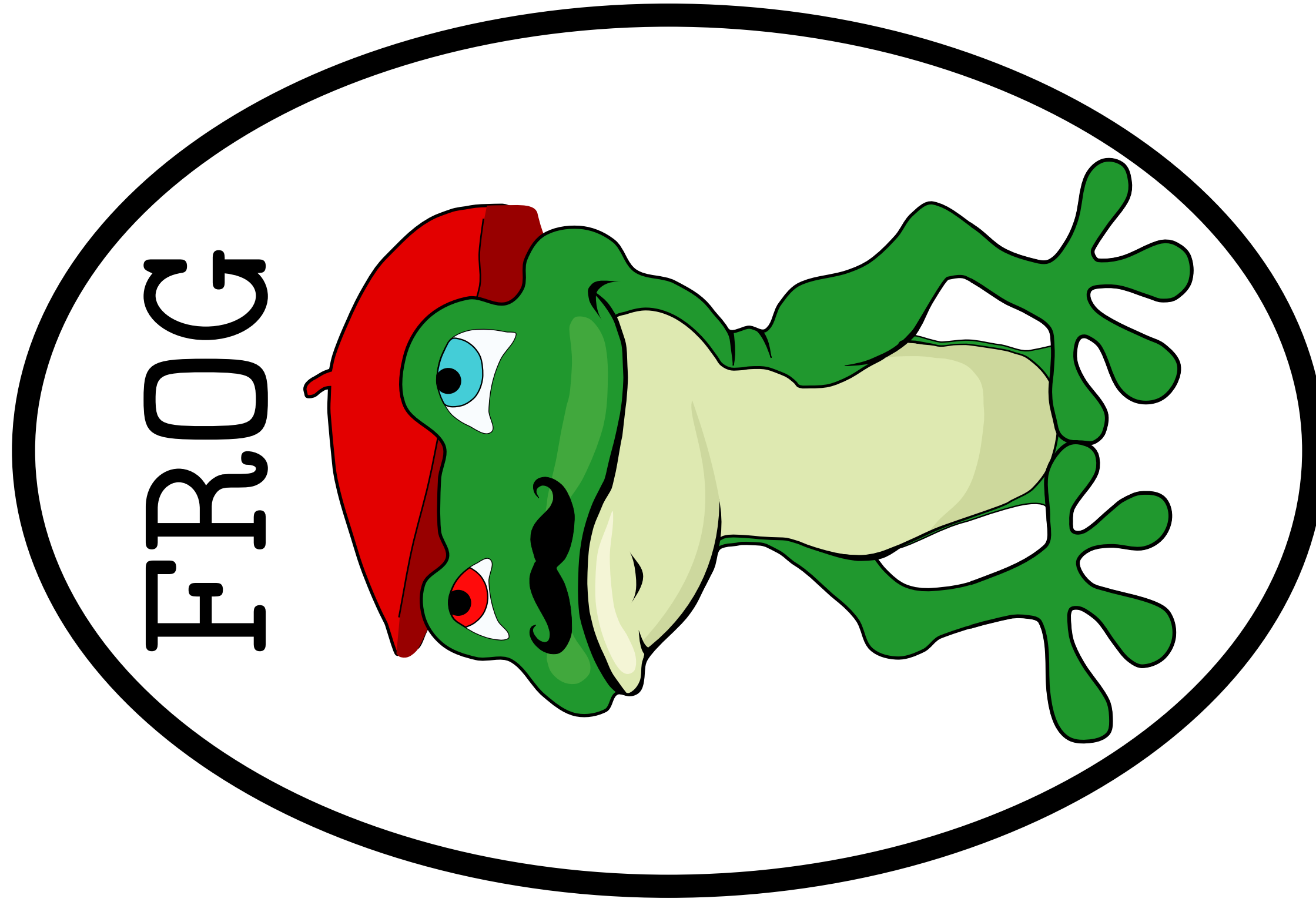
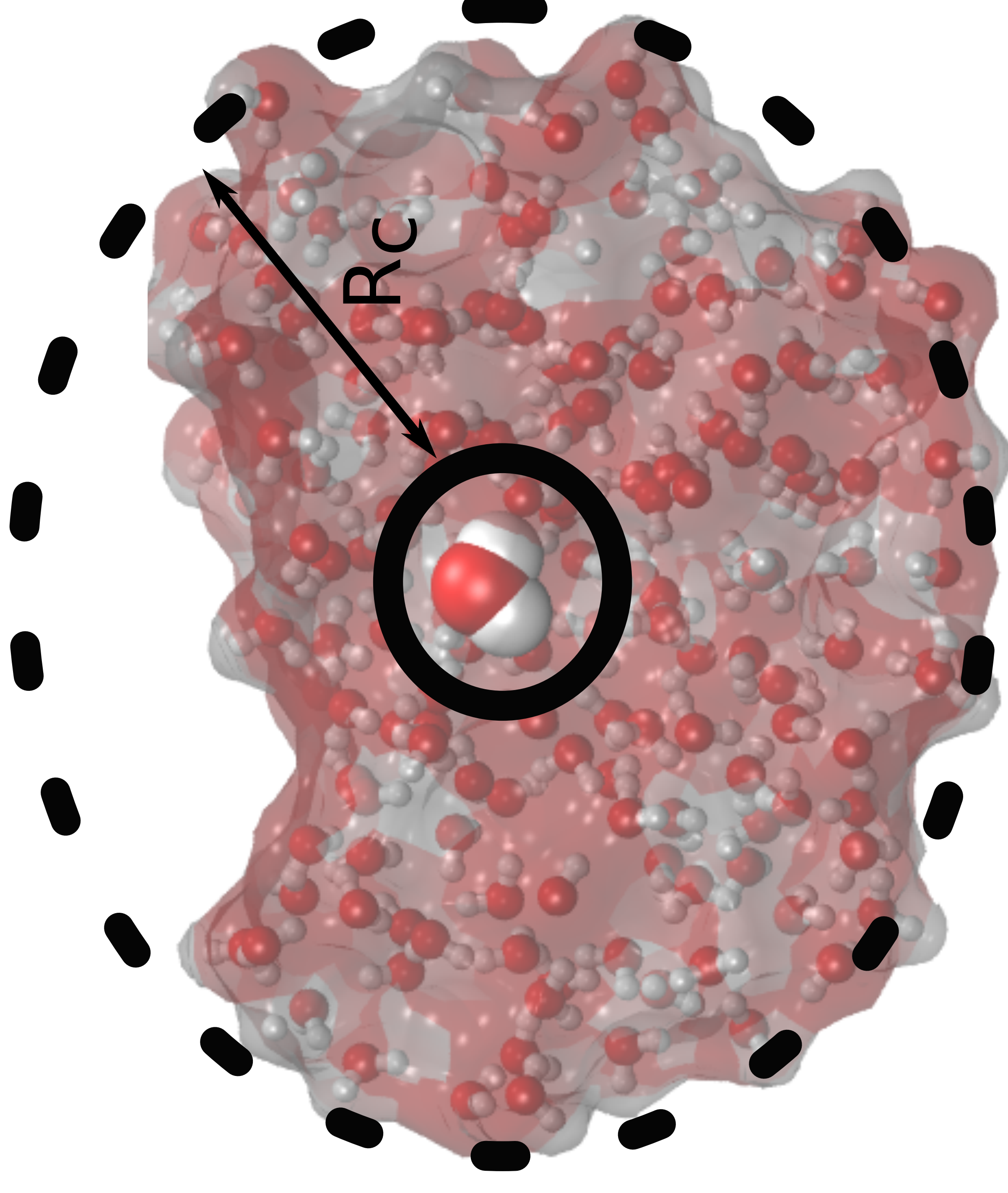


a) MD



b) Electrostatic environment



FROM molecular dynamics
to second harmonic Generation

d) Sum all molecule contribution

$$\underbrace{\chi^{(2)}(-2\omega, \omega, \omega)}_{\text{Response of the whole interface}} = \sum_{i=1}^n \underbrace{R_i R_i R_i \cdot \beta_i^{(2)}(-2\omega, \omega, \omega)}_{\text{Molecular response}}$$

(c) QM calculation

$$\beta_i^{(2)}(-2\omega, \omega, \omega)$$