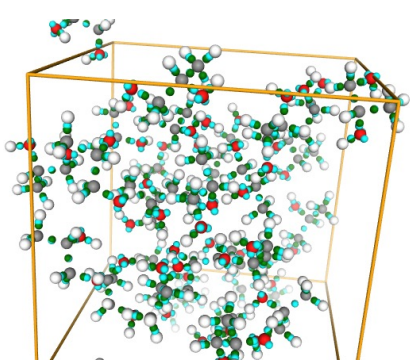
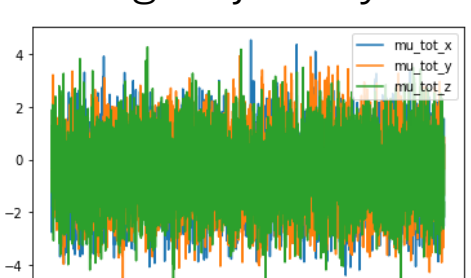
1：Trajectory from MD

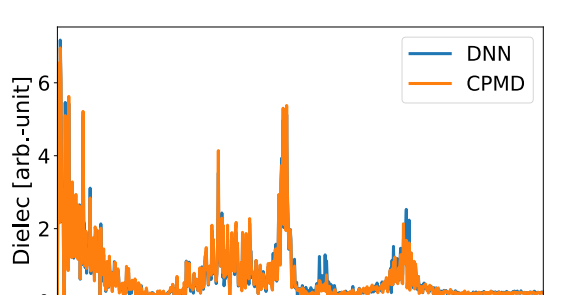


2：Dipole moment along trajectory



$$\mathbf{M} = \sum_n Z_n \mathbf{r}_n$$

3：Linear response



$$\frac{\epsilon(\omega) - \epsilon_\infty}{\epsilon_0 - \epsilon_\infty} = \int_0^\infty \left(-\frac{\langle \mathbf{M}(0) \cdot \mathbf{M}(t) \rangle}{\langle \mathbf{M}^2 \rangle} \right)' e^{-i\omega t} \mathrm{d}t$$