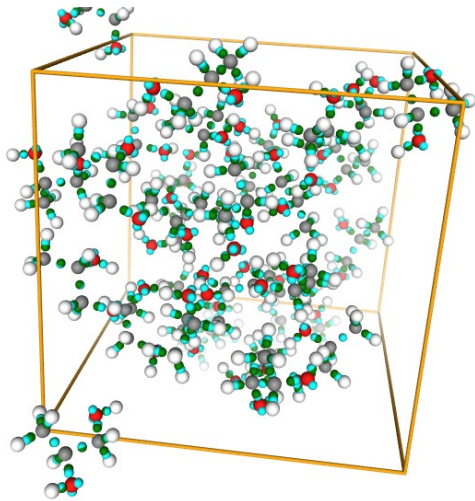
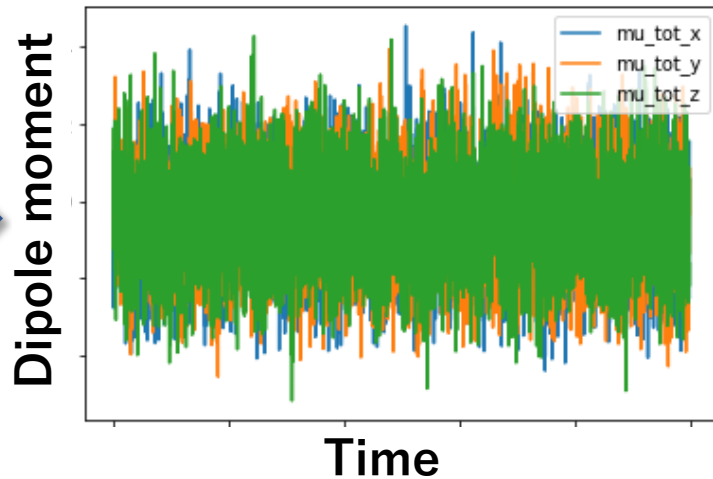


1 : MD trajectory



2 : Dipole moment

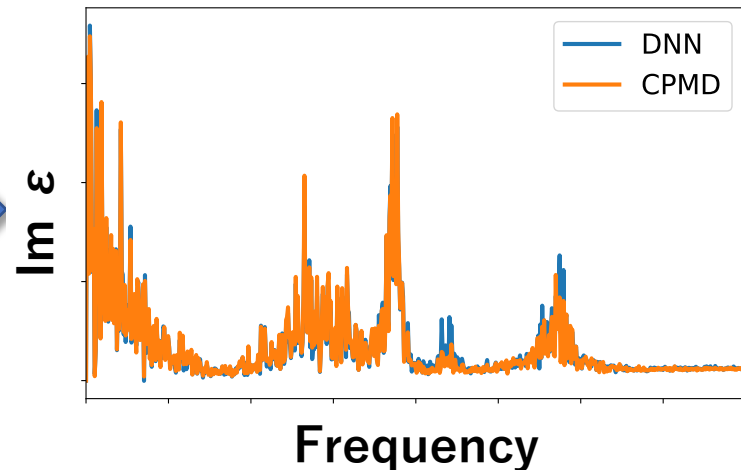


Wannier function

$$\mathbf{M} = e \sum_n Z_n \mathbf{r}_n - 2e \sum_n \mathbf{w}_n$$



3 : Dielectric function



Linear response

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