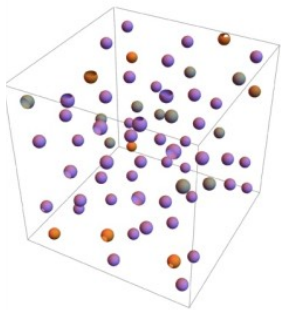
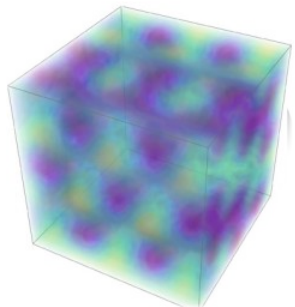
point cloud



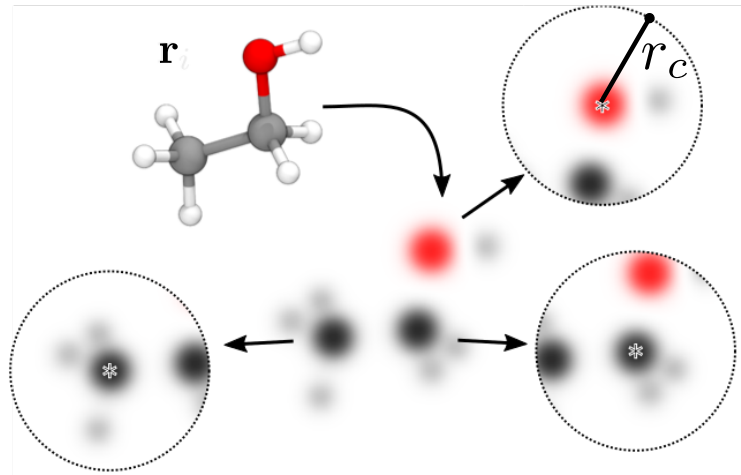
$$A = \{i | \mathbf{r}_i \in \mathbb{R}^3\}$$

atomic density

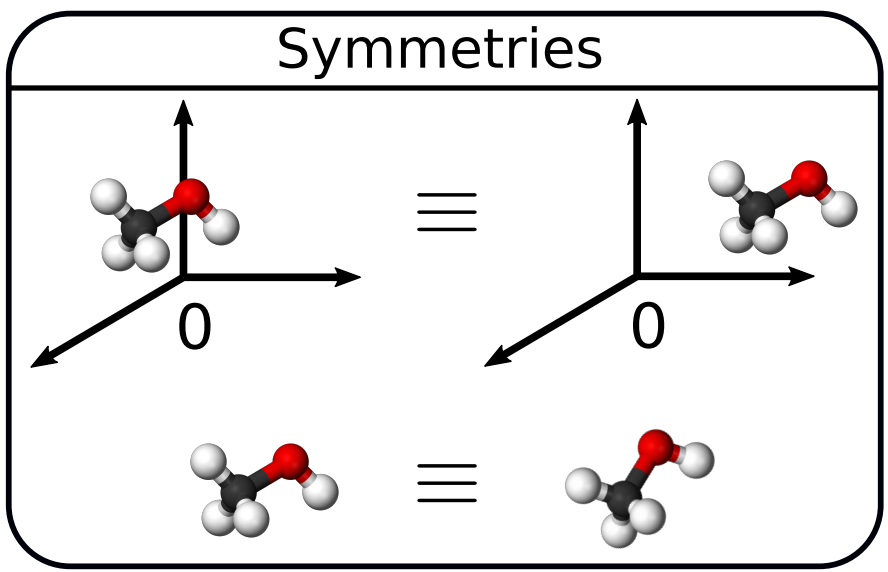


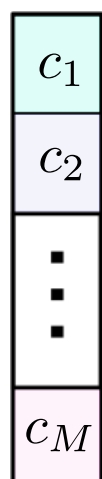
$$\rho_A(\mathbf{r}) = \sum_{i \in A} \rho(\mathbf{r} - \mathbf{r}_i)$$

split into environmental atomic densities



$$\rho_i(\mathbf{r}) = \sum_{j \in A_i} \rho(\mathbf{r} - \mathbf{r}_{ji})$$





$$c_k = \int_{\mathbb{R}^3} \rho_i^{\mathbf{q}}(\mathbf{r}) b_k(\mathbf{r}) \mathrm{d}\mathbf{r}$$

Basis expansion

on some basis set $\{b_k\}_{k=0}^{M}$