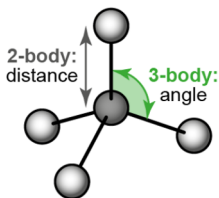
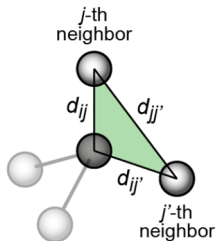
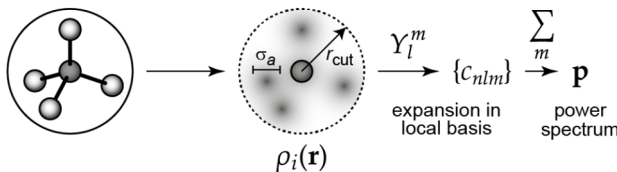


a Conventional N -body terms**b** General 3-body descriptor**c** Smooth Overlap of Atomic Positions (SOAP) descriptor**d**

sum of atomic densities

$$\rho_i(\mathbf{r}) = \rho_{ij}(\mathbf{r}) + \rho_{ij'}(\mathbf{r}) + \dots$$

$\rho_{ij}(\mathbf{r})$

$\rho_{ij'}(\mathbf{r})$

SOAP vector (power spectrum)

$$p_{nn'l} \propto \sum_{jj'} \int d\mathbf{r} d\mathbf{r}' R_n(r) R_{n'}(r') P_l(\hat{\mathbf{r}} \cdot \hat{\mathbf{r}}') \rho_{ij}(\mathbf{r}) \rho_{ij'}(\mathbf{r}')$$

individual 3-body terms

