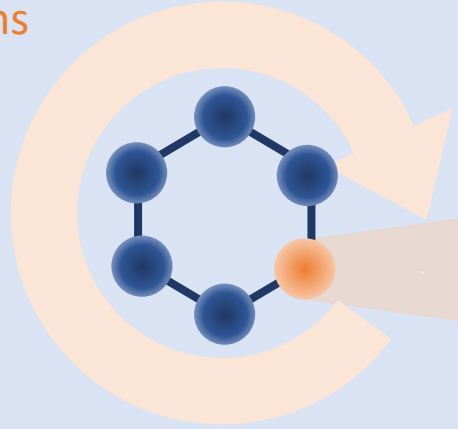
1. Loop over the atoms

Loop over unique atoms



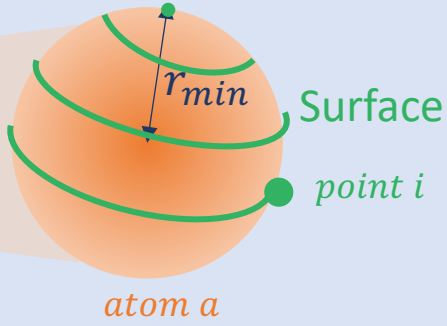
Material framework

Atom of the material

2. Sample points on the sphere

Lennard-Jones energy:

$$E_{ij}^{LJ} = \epsilon\left[\left(\frac{r_m}{r_{ij}}\right)^{12} - 2\left(\frac{r_m}{r_{ij}}\right)^{6}\right]$$



r_{min} ⟷ Distance to the minimum of the LJ potential

$-\epsilon$ Minimum of LJ potential

3. Adsorption energy calculation

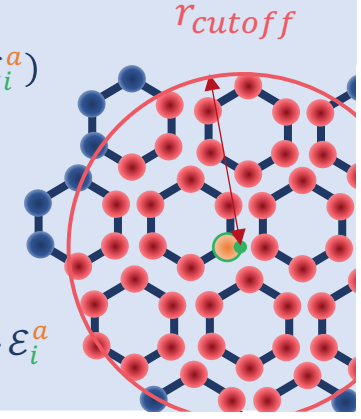
Interaction energy of an adsorbate at point 1 with the structure:

$$\mathcal{E}_i^a = E_{ia}^{LJ} + \sum_j E_{ij}^{LJ}$$

where j represents the red atoms of the structure

Boltzmann average:

$$Z = \sum_a \sum_i \exp(-\beta \mathcal{E}_i^a)$$



Approximation of the adsorption energy:

$$E_{ads} = \sum_a \sum_i \frac{\exp(-\beta \mathcal{E}_i^a)}{Z} \mathcal{E}_i^a$$