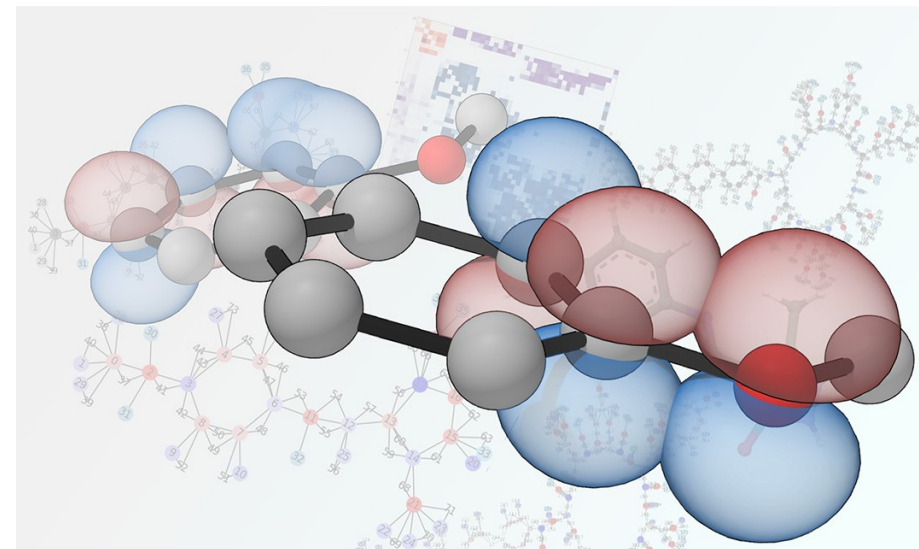


Aula 12 – Machine Learning Force Field

Ref: Artigos Citados

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$$i\hbar \frac{\partial}{\partial t} |\Psi\rangle = \hat{H} |\Psi\rangle$$

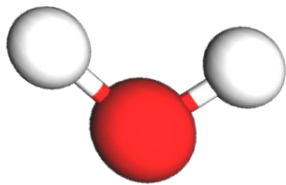
$$|\Psi\rangle = |\psi\rangle e^{-iEt/\hbar}$$

$$\hat{H} |\psi\rangle = E |\psi\rangle$$

Superfície de Energia

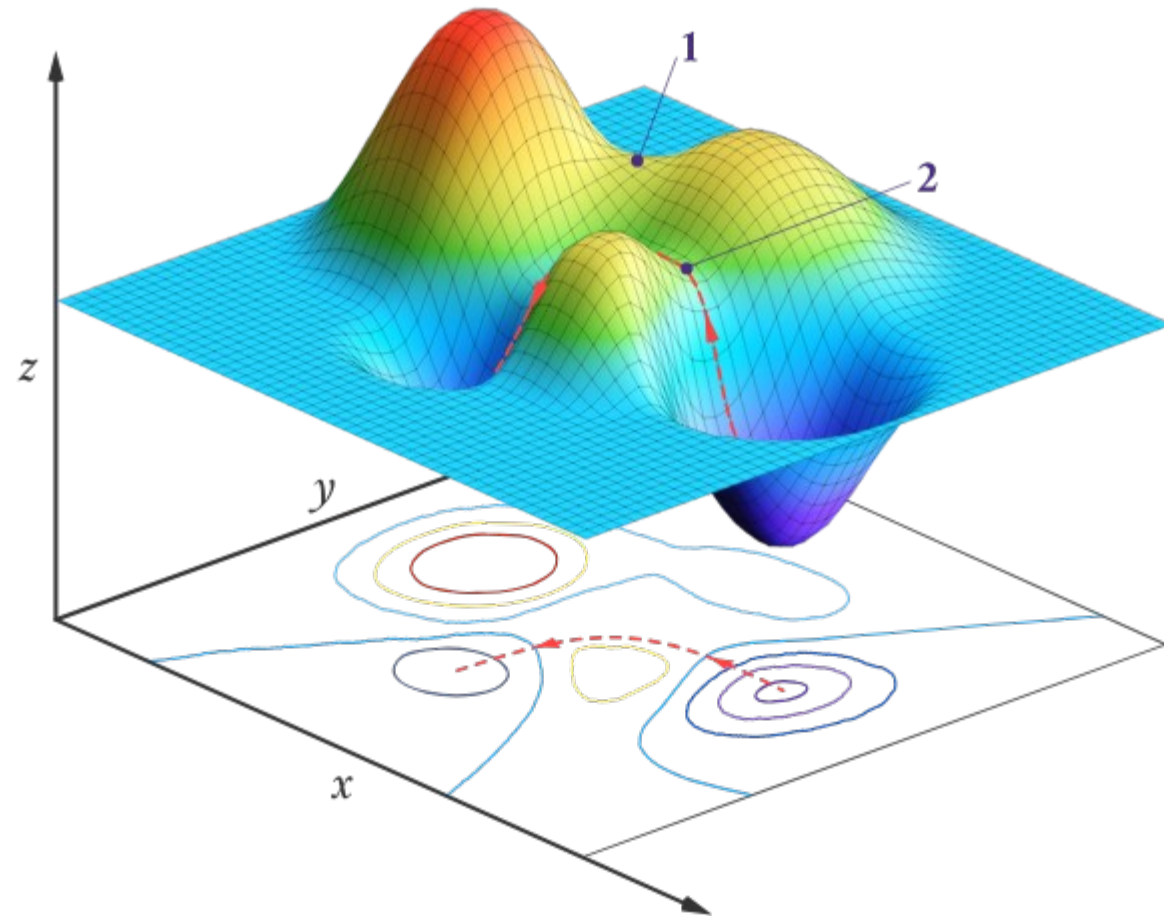
Obtido a partir de cálculos Ab Initio

- Hartree-Fock
- pós-HF;
- DFT

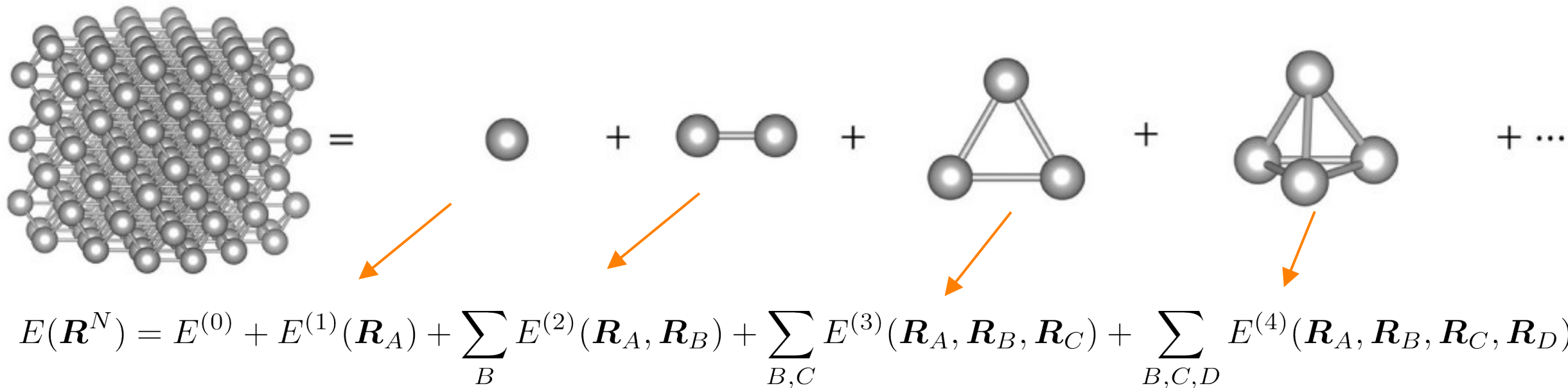


Potential Energy Surface (PES)

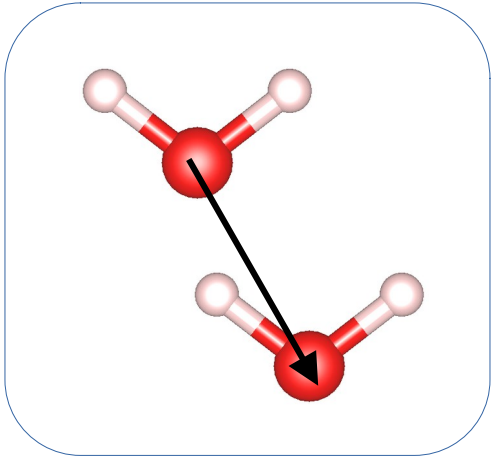
$$E(\mathbf{R}^N)$$



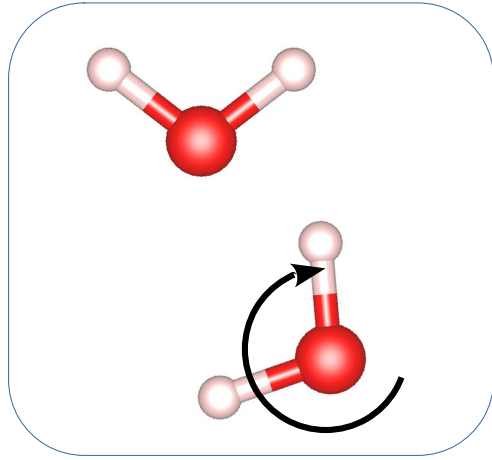
Expansão da PES em vários corpos



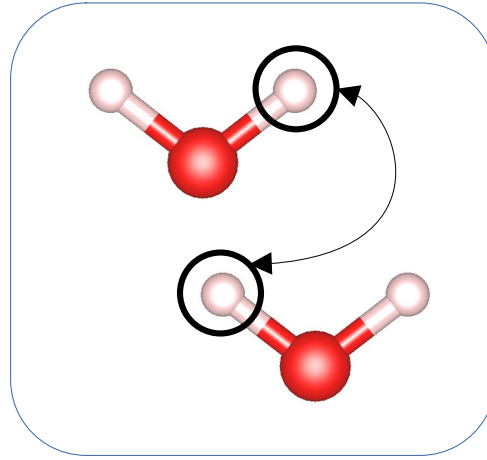
Simetrias



Translação



Rotação



Permutação

Espaço de Descritores

$$\{R_A\} \longrightarrow \{x_I\}$$

Construção de Descritores

Probabilidade de encontrar um outro átomo ao redor de i na posição \mathbf{r}

$$\rho_i(\mathbf{r}) = \sum_{j=1}^N f_{\text{cut}}(r_{ij}) g(\mathbf{r} - \mathbf{r}_j + \mathbf{r}_i)$$

Descritor radial (invariante rotacional)

$$\rho^{(2)}(r) = \frac{1}{4\pi} \int \rho_i(r\hat{\mathbf{r}}) d\hat{\mathbf{r}}$$

Descritor angular

$$\rho^{(3)}(r, s, \theta) = \iint \delta(\hat{\mathbf{r}} \cdot \hat{\mathbf{s}} - \cos \theta) \rho_i(r\hat{\mathbf{r}}) \rho_i^*(s\hat{\mathbf{s}}) d\hat{\mathbf{r}} d\hat{\mathbf{s}}$$

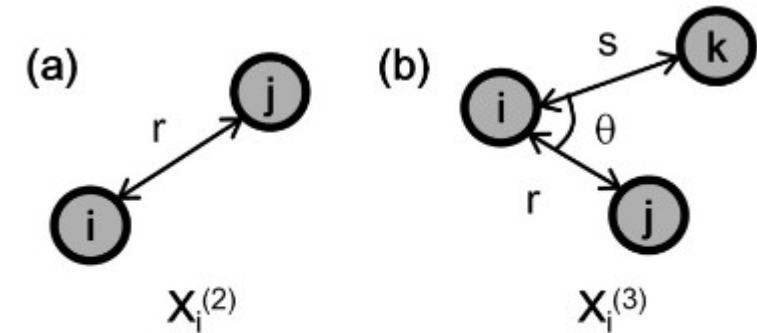


FIG. 2. (a) Radial and (b) angular descriptors.

Modelos de energia Local

Energia Local

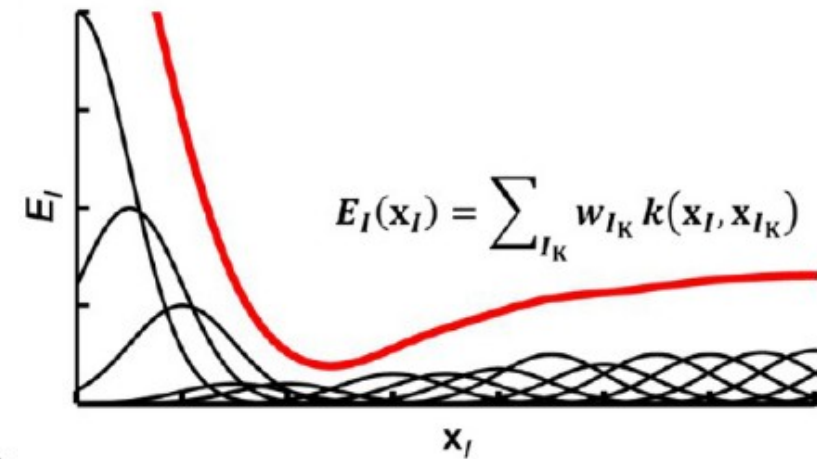
$$E(\mathbf{R}^N) = \sum_A^N E_A(\mathbf{R}^N) = \sum_I^N f(\mathbf{x}_I)$$

- Modelo de regressão Linear

$$f(\mathbf{x}_I) = \mathbf{c} \cdot \mathbf{x}_I$$

- Modelo de regressão de Kernel

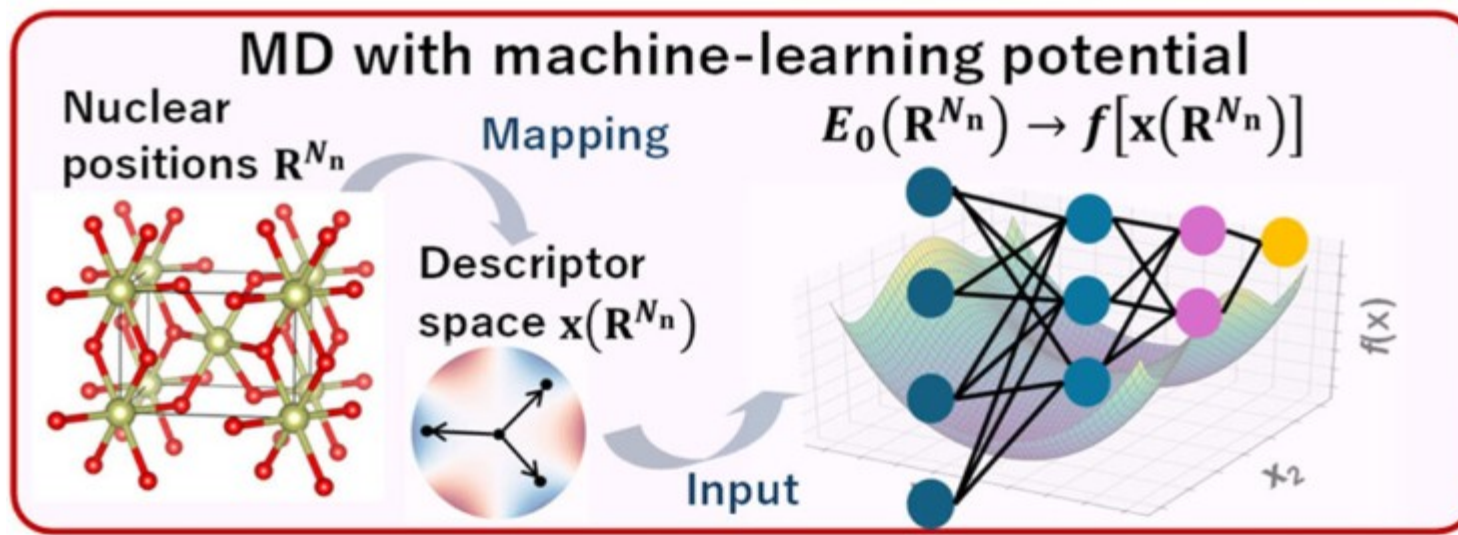
$$f(\mathbf{x}_I) = \sum_J w_J K_{IJ} \longrightarrow \mathbf{K} = \begin{bmatrix} \kappa(x_1, x_1) & \kappa(x_1, x_2) & \cdots & \kappa(x_1, x_M) \\ \kappa(x_2, x_1) & \kappa(x_2, x_2) & \cdots & \kappa(x_2, x_M) \\ \vdots & \vdots & \ddots & \vdots \\ \kappa(x_M, x_1) & \kappa(x_M, x_2) & \cdots & \kappa(x_M, x_M) \end{bmatrix}.$$



Exemplo de Kernel

$$E(\mathbf{R}^N) = \sum_A E_A(\mathbf{R}^N) = \sum_I^N \sum_J^M w_J K(\mathbf{X}_I, \mathbf{X}_J)$$

$$K(\mathbf{X}_I, \mathbf{X}_J) = \beta^{(2)}(\mathbf{X}_I^{(2)} \cdot \mathbf{X}_J^{(2)}) + \beta^{(3)}(\mathbf{X}_I^{(3)} \cdot \mathbf{X}_J^{(3)})^\zeta$$



PyAMFF: Python Atom-Centered Machine Learning Force Field

