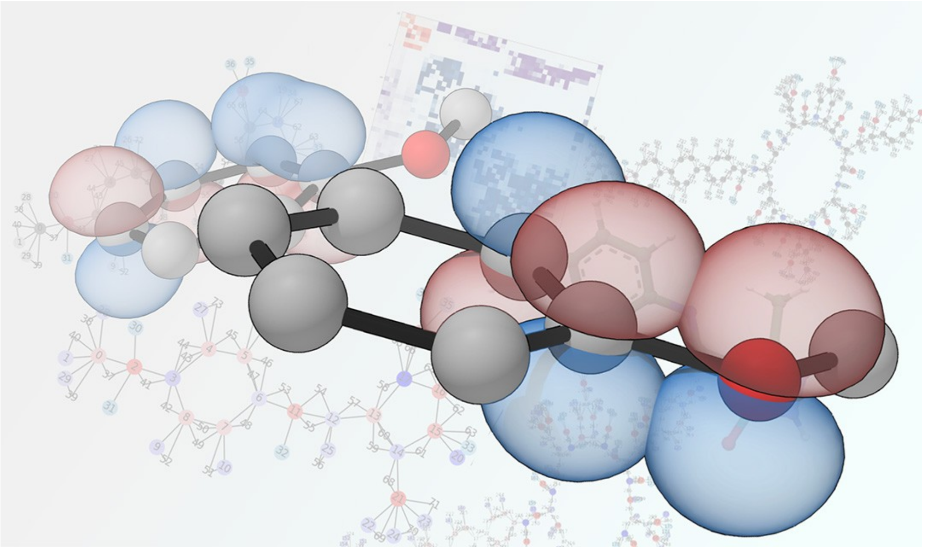
Aula 12 – Machine Learning Force Field



Ref: Artigos Citados

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

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

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

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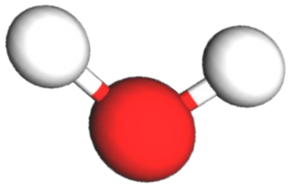
Superfície de Energia Potencial

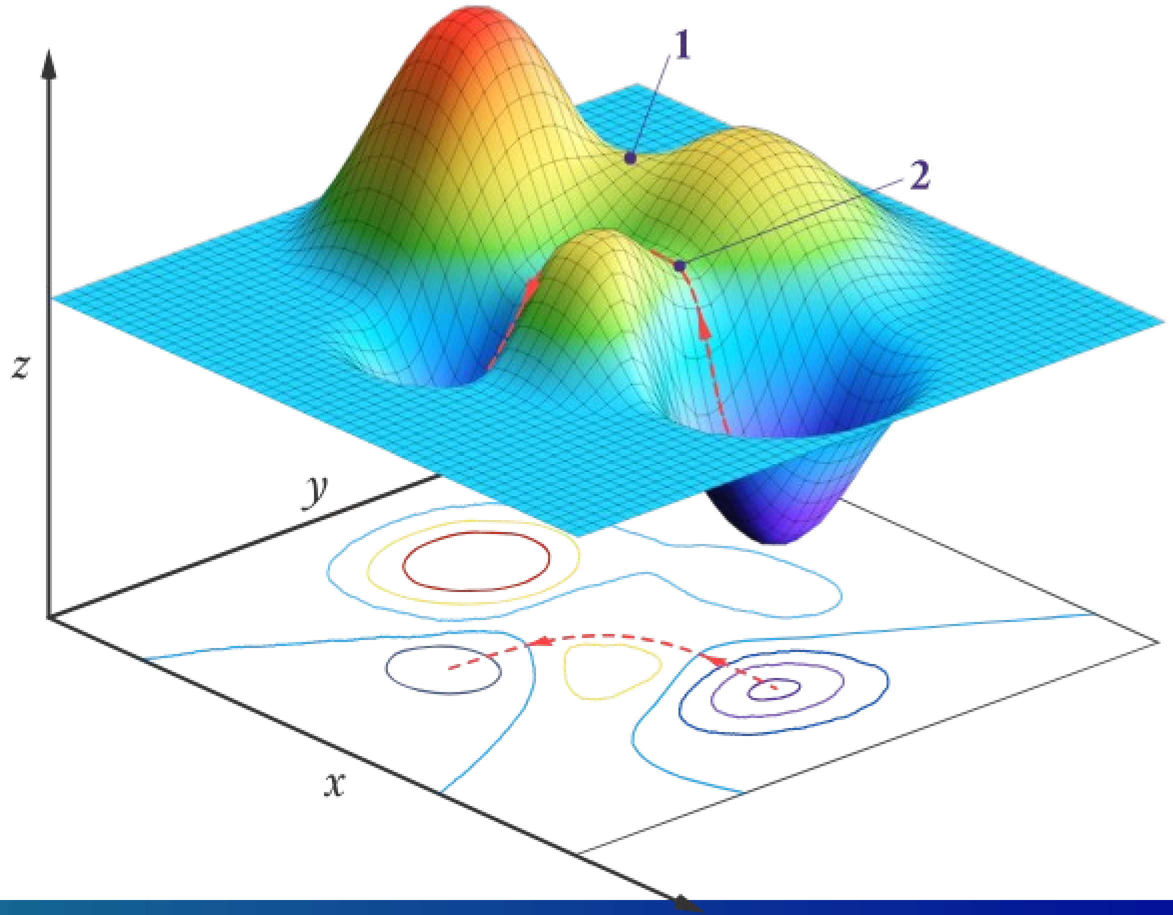
Potential Energy Surface (PES)

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

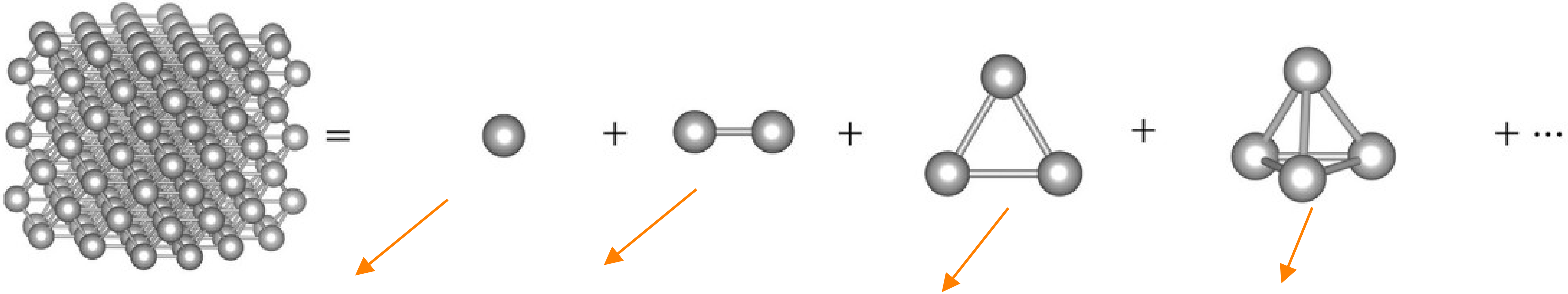
Obtido a partir de cálculos Ab Initio

- Hartree-Fock
- pós-HF;
- DFT





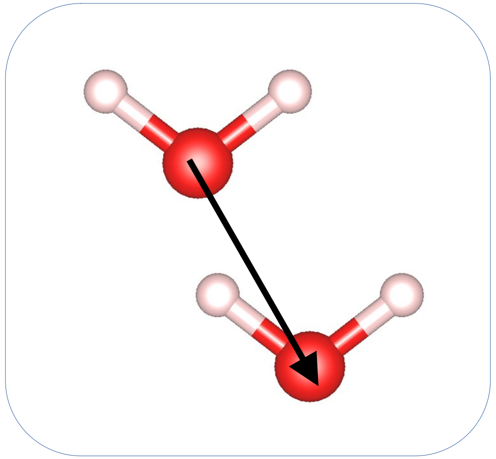
Expansão da PES em vários corpos



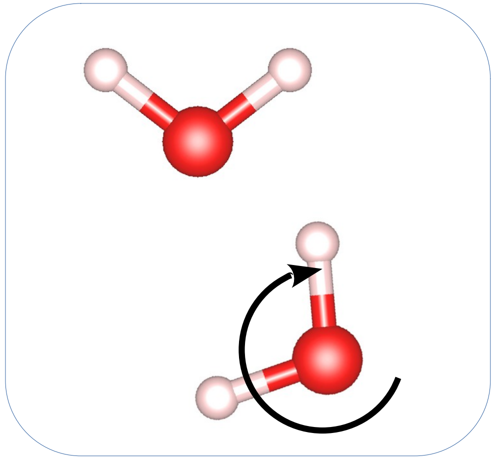
$$E(\boldsymbol{R}^N) = E^{(0)} + \sum_{A} E^{(1)}(\boldsymbol{R}_A) + \sum_{A,B} E^{(2)}(\boldsymbol{R}_A, \boldsymbol{R}_B) + \sum_{A,B,C} E^{(3)}(\boldsymbol{R}_A, \boldsymbol{R}_B, \boldsymbol{R}_C) + \sum_{A,B,C,D} E^{(4)}(\boldsymbol{R}_A, \boldsymbol{R}_B, \boldsymbol{R}_C, \boldsymbol{R}_D) + \ldots$$

Jinnouchi, R., & Minami, S. (2025). ACS Nano, 19(25), 22600–22644. https://doi.org/10.1021/acsnano.5c05553

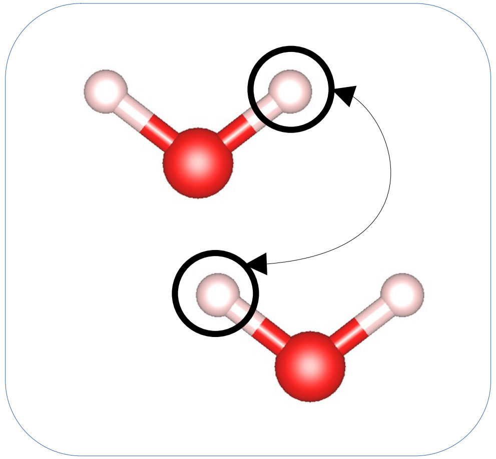
Simetrias



Translação



Rotação



Permutação

Espaço de Descritores

$$\{\boldsymbol{R}_A\} \longrightarrow \{\boldsymbol{x}_I\}$$

Construção de Descritores

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

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

Descritor radial (invariante rotacional)

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

Descritor angular

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

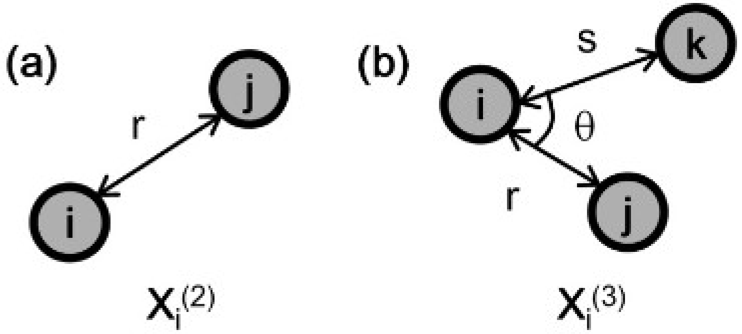


FIG. 2. (a) Radial and (b) angular descriptors.

Jinnouchi, R. *et al* (2019). Physical Review Letters, 122(22), 225701. https://doi.org/10.1103/PhysRevLett.122.225701

Modelos de energia Local

Energia Local

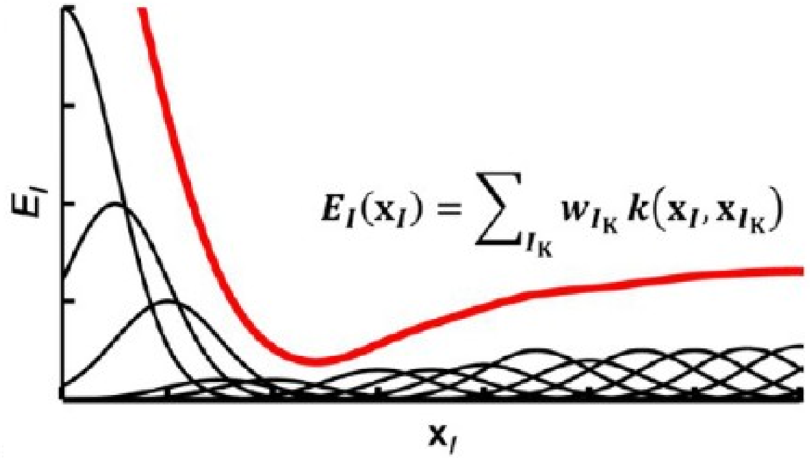
$$E(\boldsymbol{R}^N) = \sum_A^N E_A(\boldsymbol{R}^N) = \sum_I^N f(\boldsymbol{x}_I)$$

- Modelo de regressão Linear

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

- Modelo de regressão de Kernel

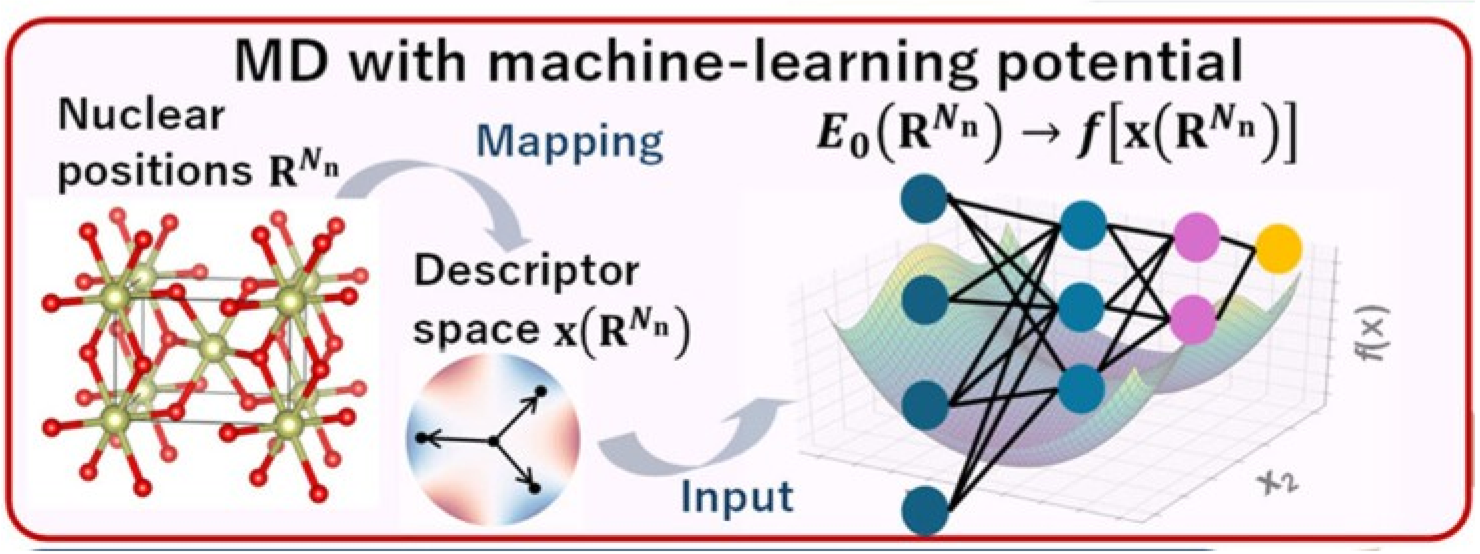
$$f(\boldsymbol{x}_I) = \sum_J w_J K_{IJ} \longrightarrow \mathbf{K} = \begin{bmatrix} \kappa(x_1,x_1) & \kappa(x_1,x_2) & \cdots & \kappa(x_1,x_M) \\ \kappa(x_2,x_1) & \kappa(x_2,x_2) & \cdots & \kappa(x_2,x_M) \\ \vdots & \vdots & \ddots & \vdots \\ \kappa(x_M,x_1) & \kappa(x_M,x_2) & \cdots & \kappa(x_M,x_M)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



Exemplo de Kernel

$$E(\boldsymbol{R}^N) = \sum_{A}^{N} E_A(\boldsymbol{R}^N) = \sum_{I}^{N} \sum_{J}^{M} w_J K(\boldsymbol{X}_I, \boldsymbol{X}_J)$$

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



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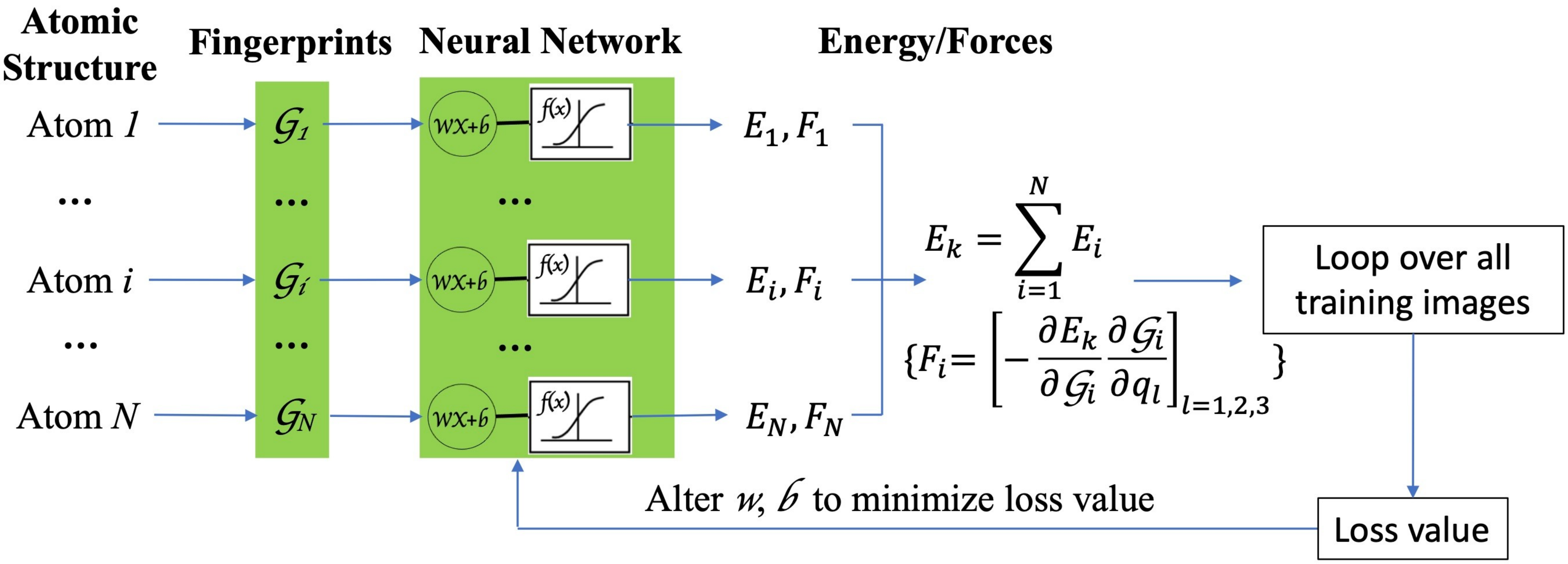
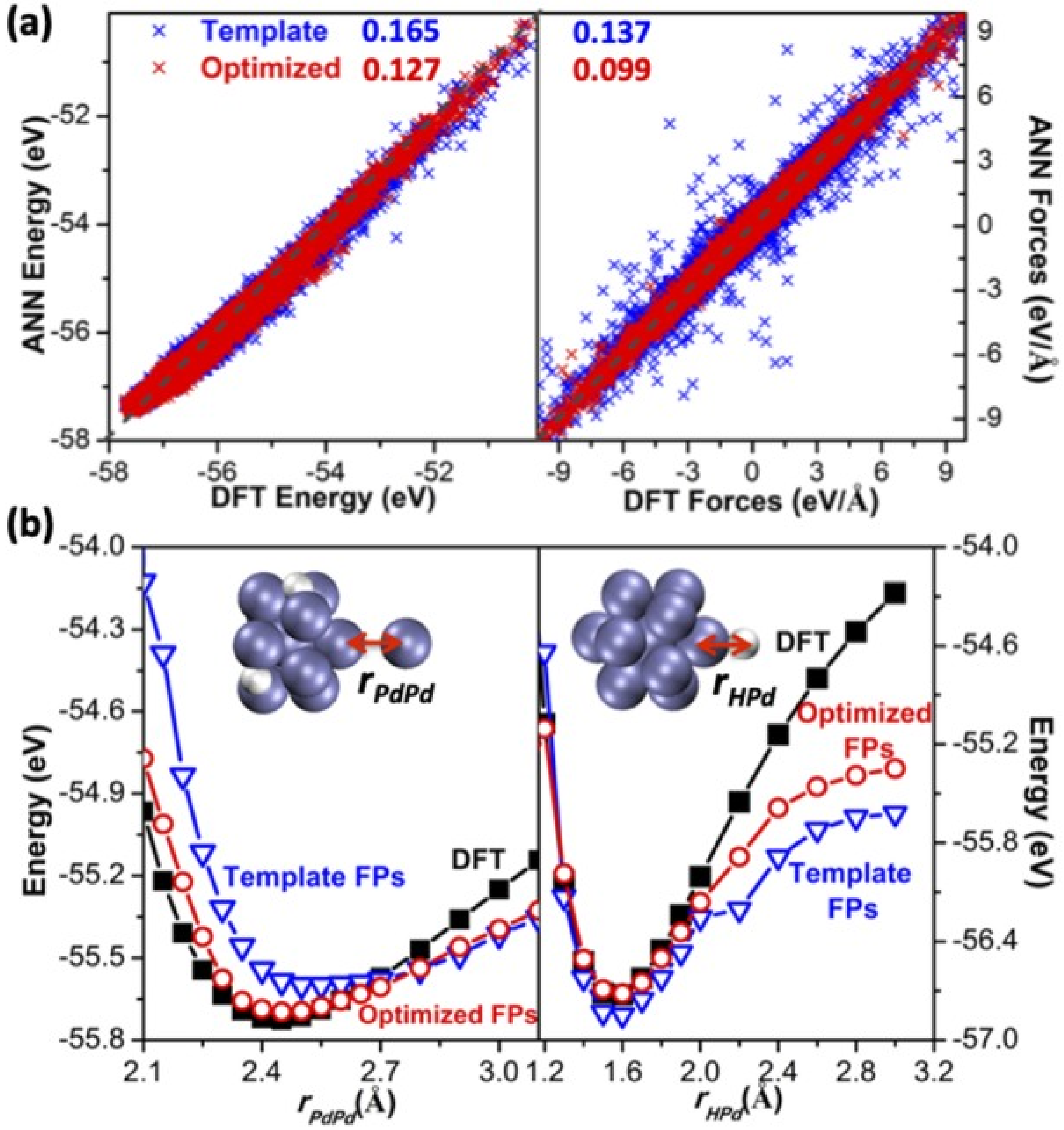
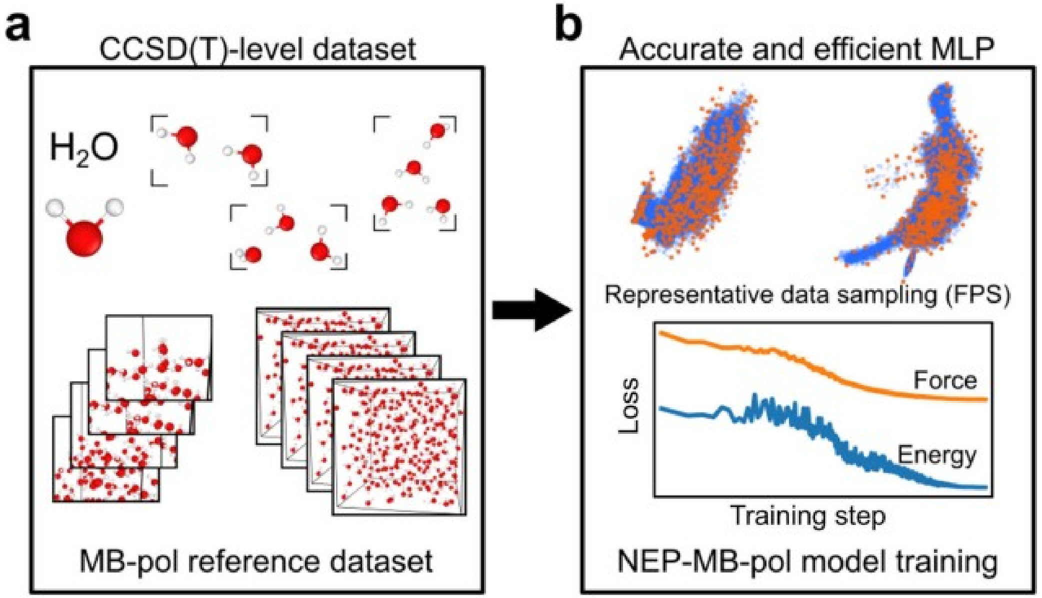
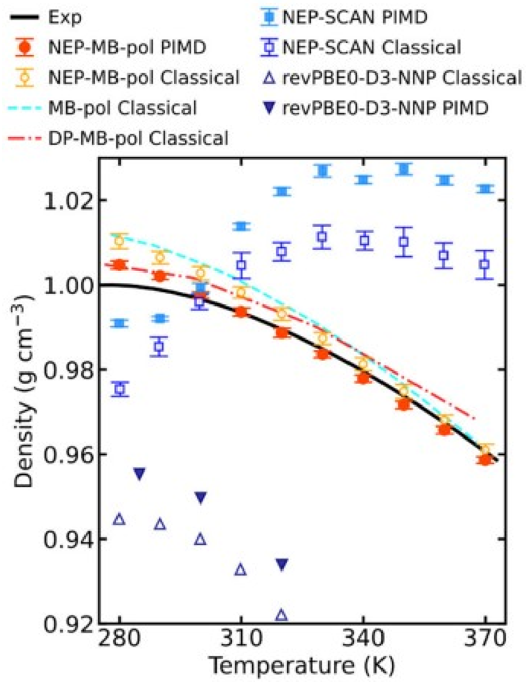
PyAMFF: Python Atom-Centered Machine Learning Force Field

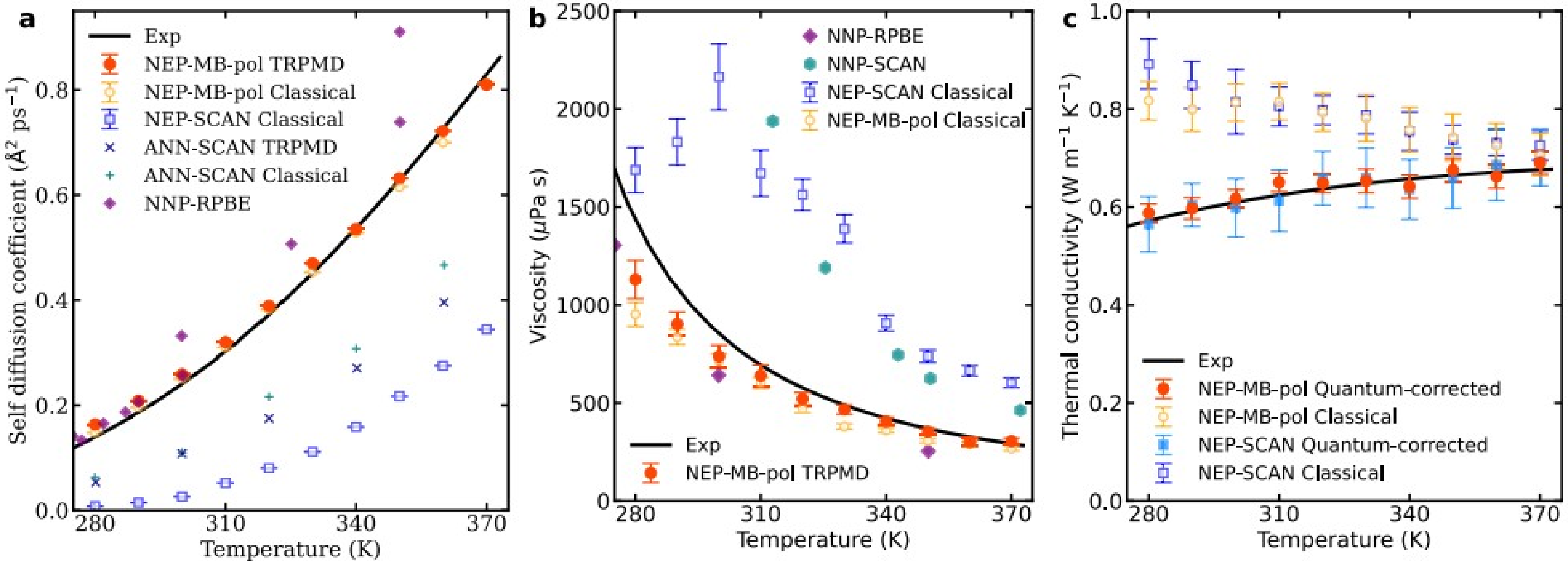




Li, L., Li, H., Seymour, I. D., Koziol, L., & Henkelman, G. (2020). The Journal of Chemical Physics, 152(22), 224102. https://doi.org/10.1063/5.0007391







Li, L., Li, H., Seymour, I. D., Koziol, L., & 3/5.
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