انجمن فیزیک ایران

دانشگاه زابل

High-dimensional Neural Network potential

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2ND WORKSHOP ON MACHINE LEARNING IN PHYSICS: APPLICATIONS IN CONDENSED MATTER PHYSICS

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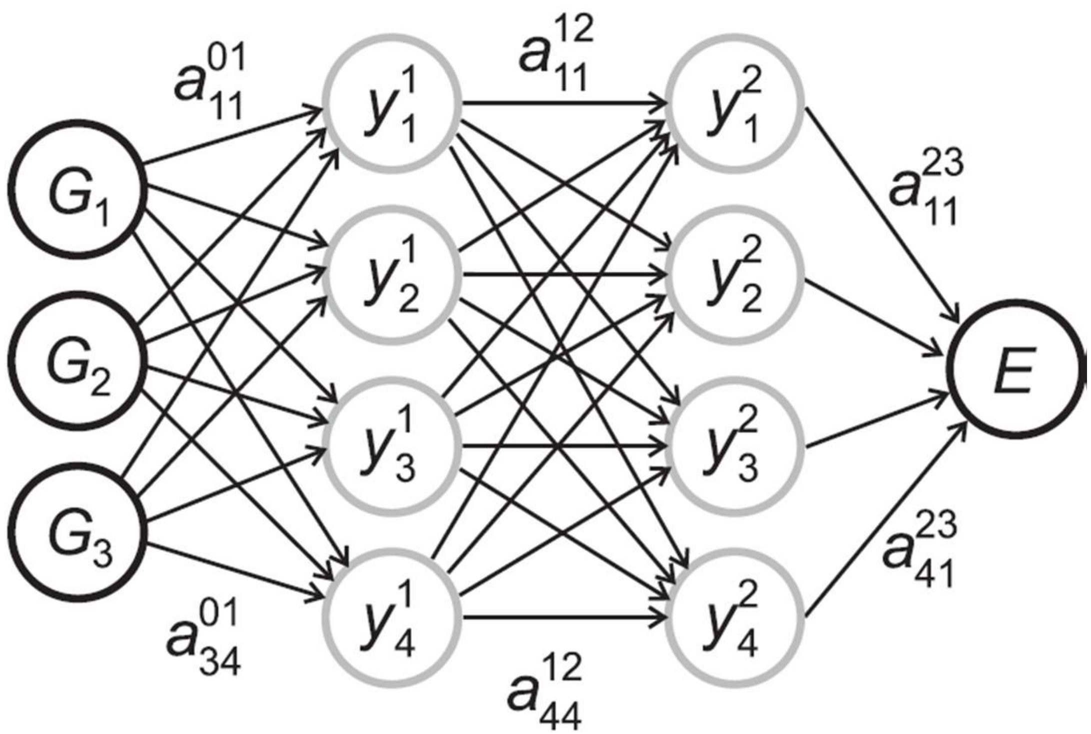
Outline

- Limitations of single NN potentials.
- Structure of high-dimensional NN potentials.
- Symmetry functions for high-dimensional NN potentials.
- Properties of symmetry functions.
- Functional form of symmetry functions.
- Some notes in constructing symmetry functions set.

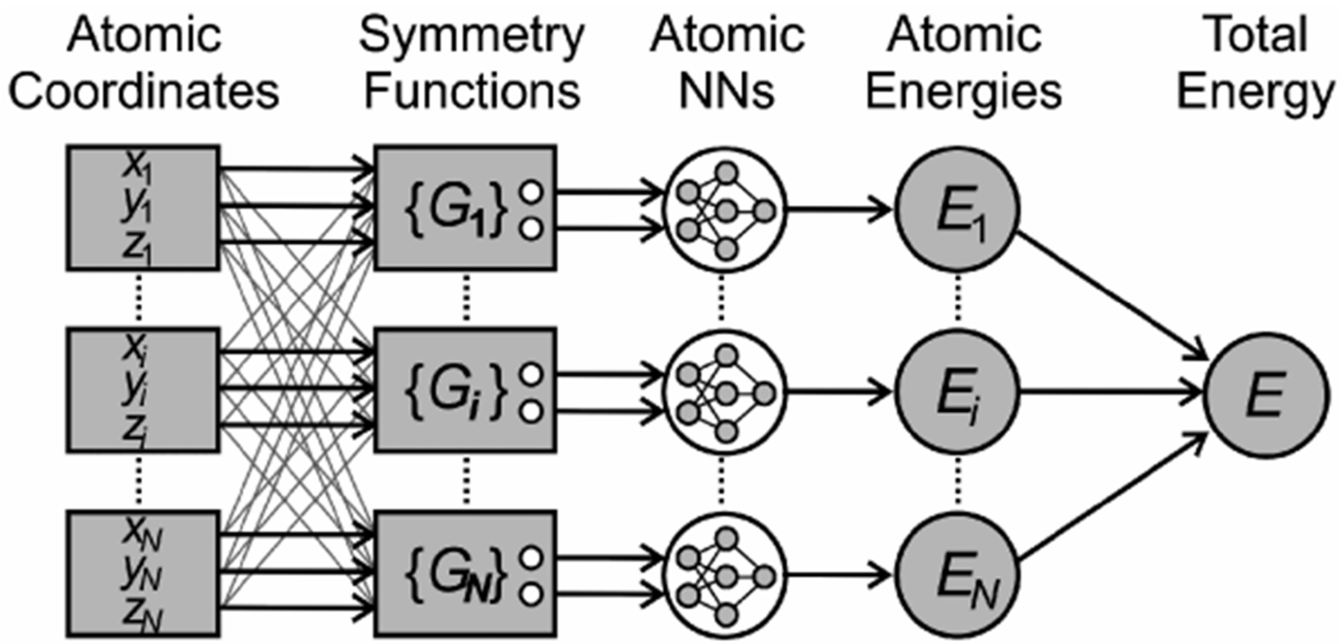
Limitations of single Neural Network potential

- **Restriction to low dimensional system.**
- **Only applicable to the system size that has been used for its construction.**
- **Challenge in the incorporation invariance with respect to:**
  - **Translation**
  - **Rotation**
  - **Permutation**



Structure of high-dimensional NN potentials

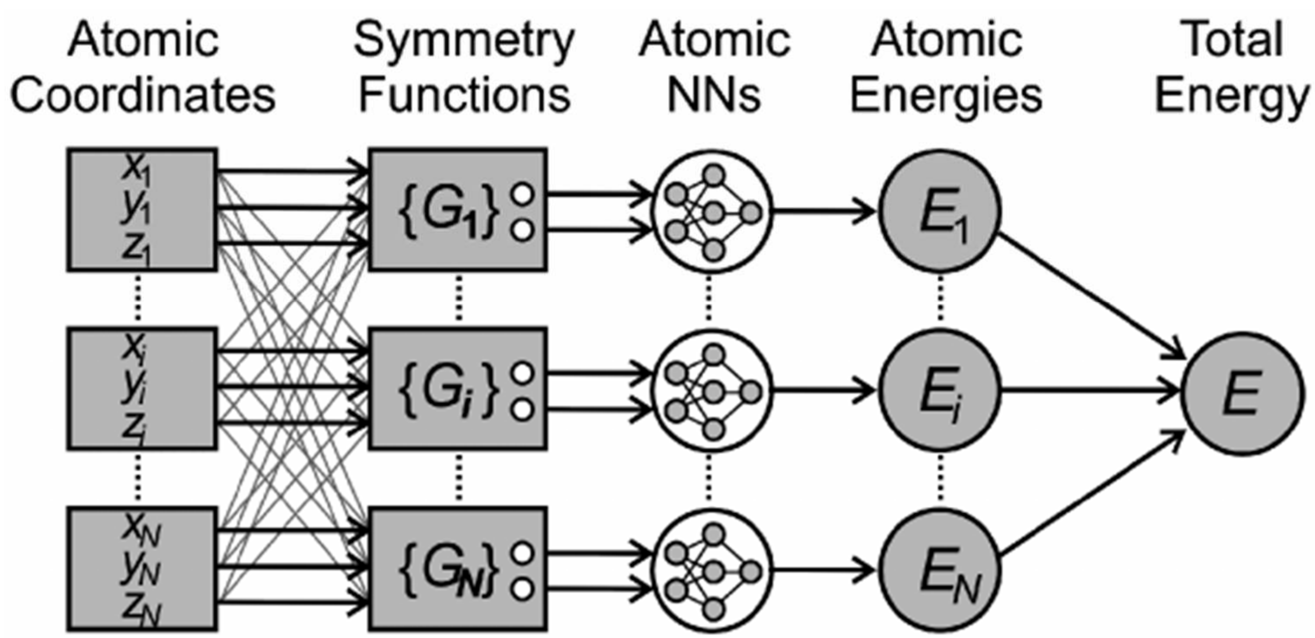
The central idea is using a set of atomic NNs instead of a single NN :



$$E = \sum_{i=1}^{N_{atom}} E_i$$

- ➢ **Each line represents one atom i.**
- ➢ **Same atomic NN topology and weight parameters for same chemical species.**
- ➢ **The {Gi} set describe the atomic environment of atom i within a cutoff radius Rc (6 to 10 Å).**

Advantages of high-dimensional NN potentials



- Applicable to arbitrary numbers of atoms.
- Invariant with respect to permutations of the order of the atoms.
- Invariant with respect to rotation and translation of the system.
- Well suited for parallel implementations.

Symmetry functions for high-dimensional NN potentials

Requirements:

(a) Be continuous in value and slope.

(b) Be invariant with respect to translation and rotation of the system.

(c) Be invariant with respect to permutations of chemically equivalent atoms in the atomic environments.

(d) Constant number of symmetry functions in the $\{G_i\}$ set.

(e) Decay to zero for large interatomic distances .

(f) Provide a unique description of the atomic environments

Construction of the symmetry functions.

Cutoff function:

$$f_{c,1}(R_{ij}) = \begin{cases} 0.5. \left[\cos\left(\frac{\pi R_{ij}}{R_c}\right) + 1\right] & \text{for } R_{ij} \leqslant R_c \\ 0 & \text{for } R_{ij} > R_c \end{cases}$$

JChemPhys-2011-V134-074106-Behler

$$f_{c,2}(R_{ij}) = \begin{cases} \tanh^3\left[1 - \frac{R_{ij}}{R_c}\right] & \text{for } R_{ij} \leqslant R_c \\ 0 & \text{for } R_{ij} > R_c. \end{cases}$$

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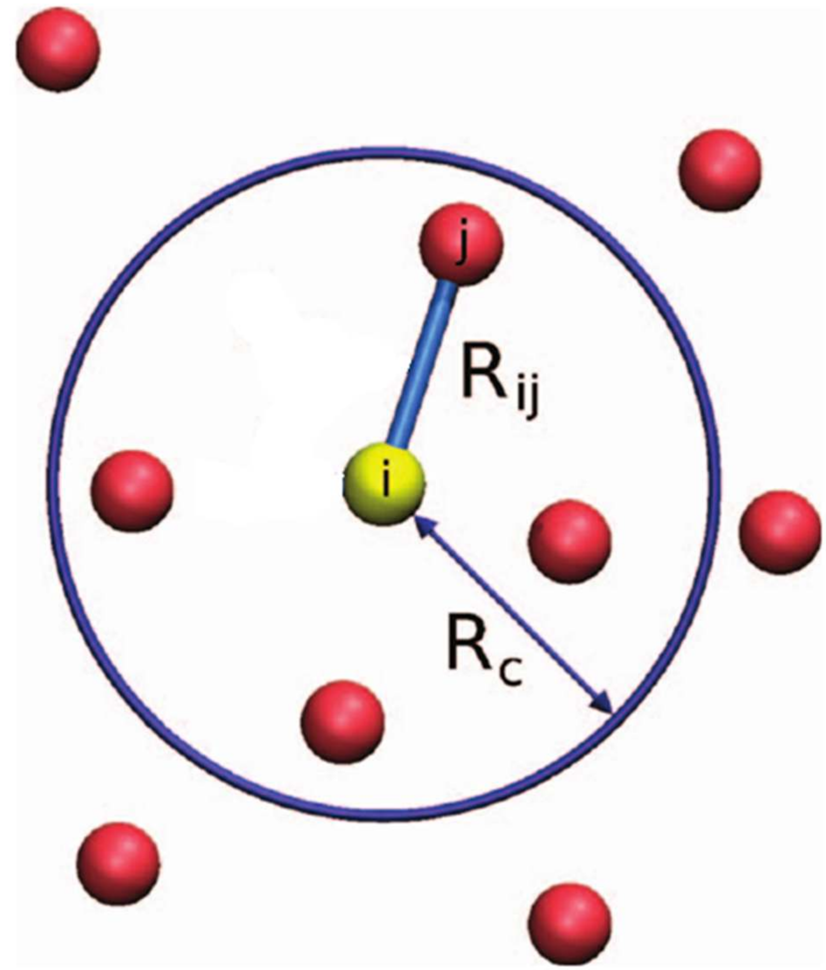
$$f_{c,3}(R_{ij}) = \begin{cases} \left(1 - \frac{R_{ij}^2}{R_c^2}\right)^3 & \text{for } R_{ij} \leqslant R_c \\ 0 & \text{for } R_{ij} > R_c \end{cases}$$

PhysRevB-2015-V92-045131-Ghasemi

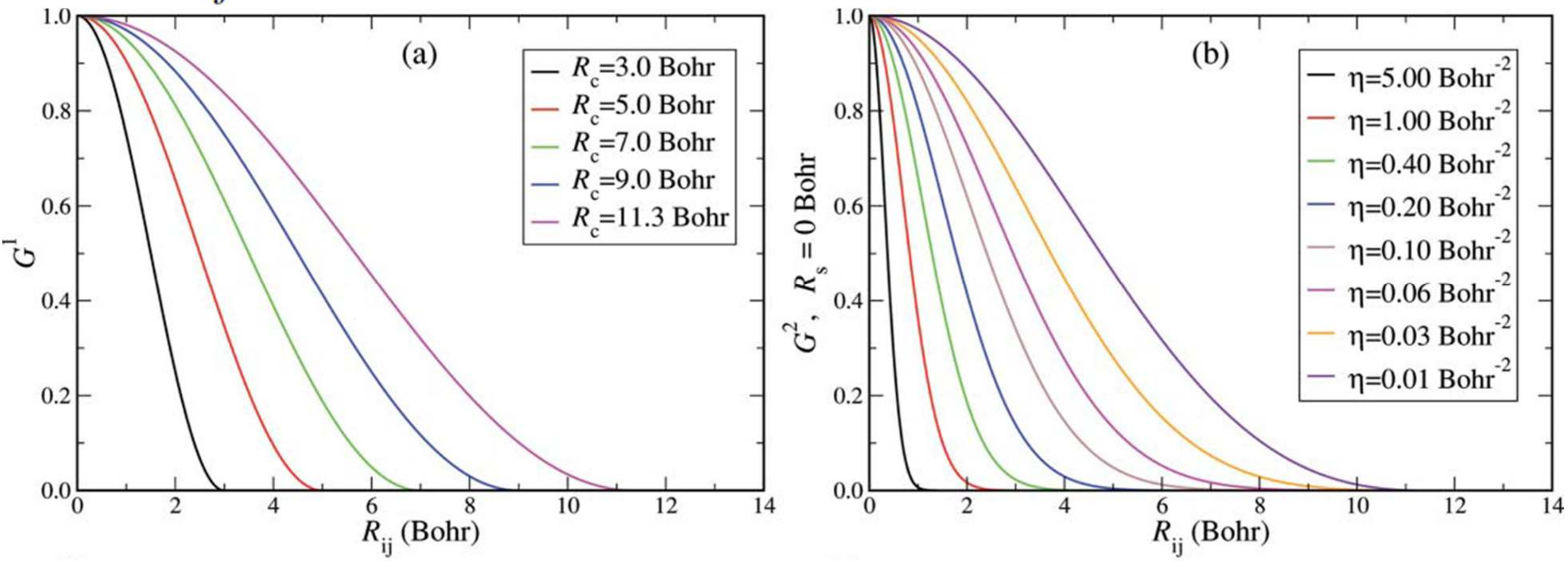


Construction of the symmetry functions.

Radial functions:

$$G_i^1 = \sum_j f_c(R_{ij})$$

$$G_i^2 = \sum_j e^{-\eta(R_{ij}-R_s)^2} \cdot f_c(R_{ij})$$



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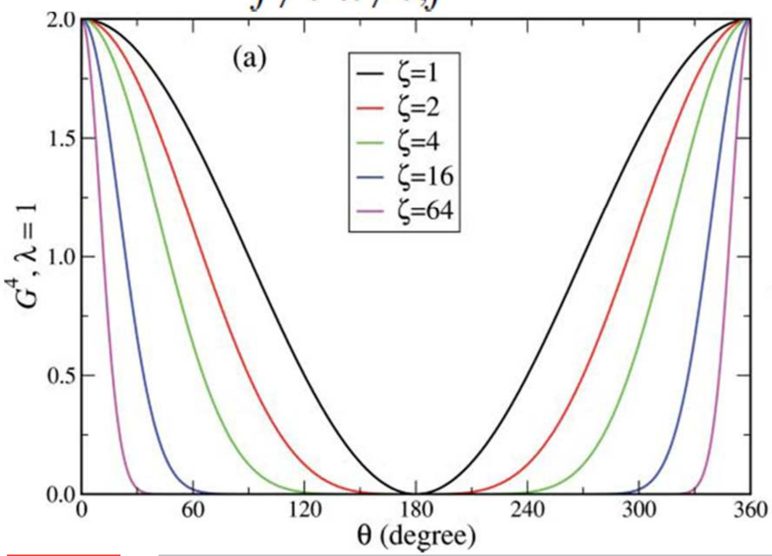
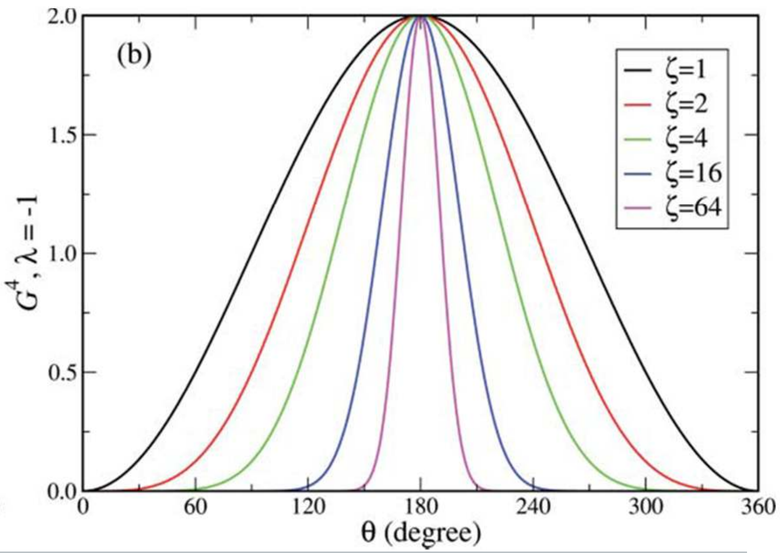
Construction of the symmetry functions.

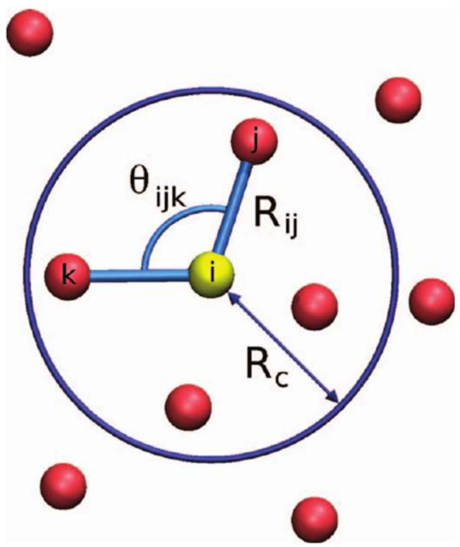
Angular functions :

$$G_i^4 = 2^{1-\zeta} \sum_{j \neq i} \sum_{k \neq i,j} \Big[\left(1 + \lambda \cdot \cos\theta_{ijk}\right)^{\zeta} \times e^{-\eta\left(R_{ij}^2 + R_{ik}^2 + R_{jk}^2\right)} \cdot f_c\left(R_{ij}\right) \cdot f_c\left(R_{ik}\right) \cdot f_c\left(R_{jk}\right) \Big]$$

$$G_i^5 = 2^{1-\zeta} \sum_{j \neq i} \sum_{k \neq i,j} \Big[\left(1 + \lambda \cdot \cos\theta_{ijk}\right)^{\zeta} \cdot e^{-\eta\left(R_{ij}^2 + R_{ik}^2\right)} \cdot f_c\left(R_{ij}\right) \cdot f_c\left(R_{ik}\right) \Big]$$







Important properties of symmetry functions

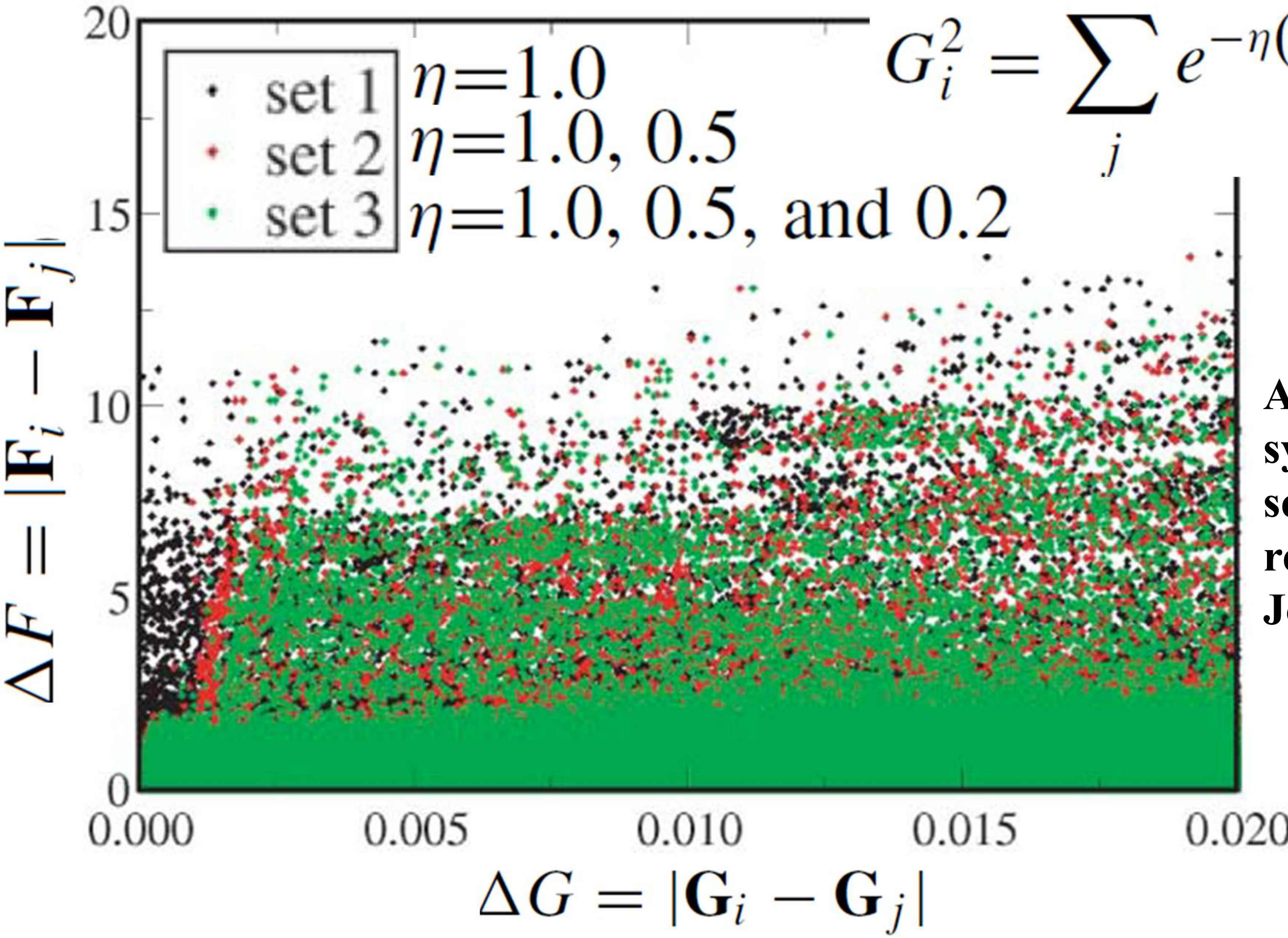
- Rotational, translational and permutation invariance
- Provide a unique description of the atomic environment.
- Constant number of function values
- Physically they are related to effective coordination numbers

Some notes in constructing symmetry functions set

- ❑ Compute many symmetry function candidates for the various phases of interest and select the symmetry functions which best differentiate between the phases, i.e., those corresponding to small overlaps.
- ❑ Determine the derivative of the output of the network with respect to its input and eliminates the input nodes with derivative close to zero.
- ❑ For each symmetry function, analyze the range of values present in the data set. If the range of values, is too small the symmetry function is not suitable.
- ❑ If there is a high correlation between the values of two symmetry functions for all atoms in the training, the symmetry functions are (close to) linearly dependent.

Some notes in constructing symmetry functions set

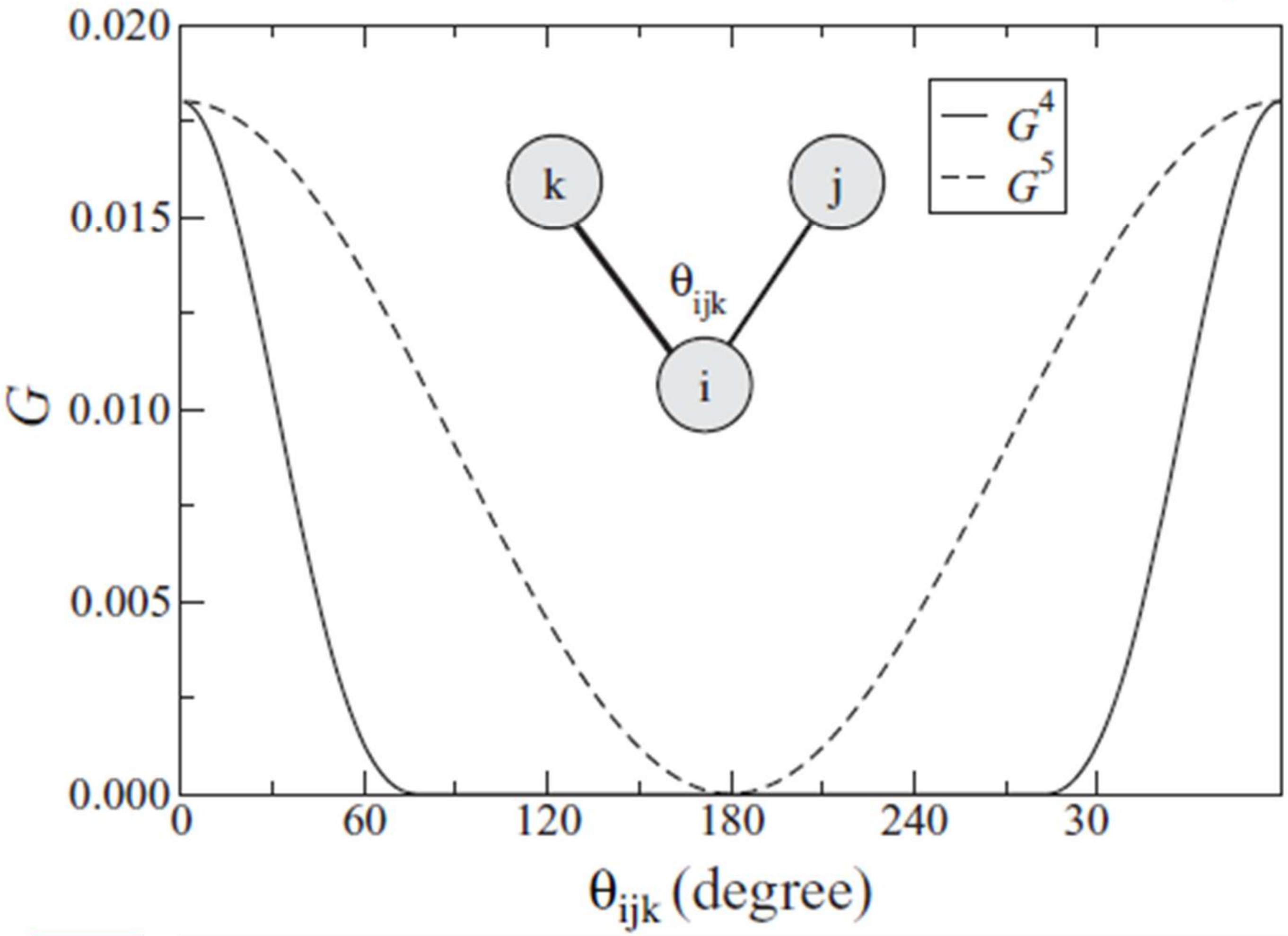
$$G_i^2 = \sum_j e^{-\eta(R_{ij}-R_s)^2} \cdot f_c(R_{ij})$$

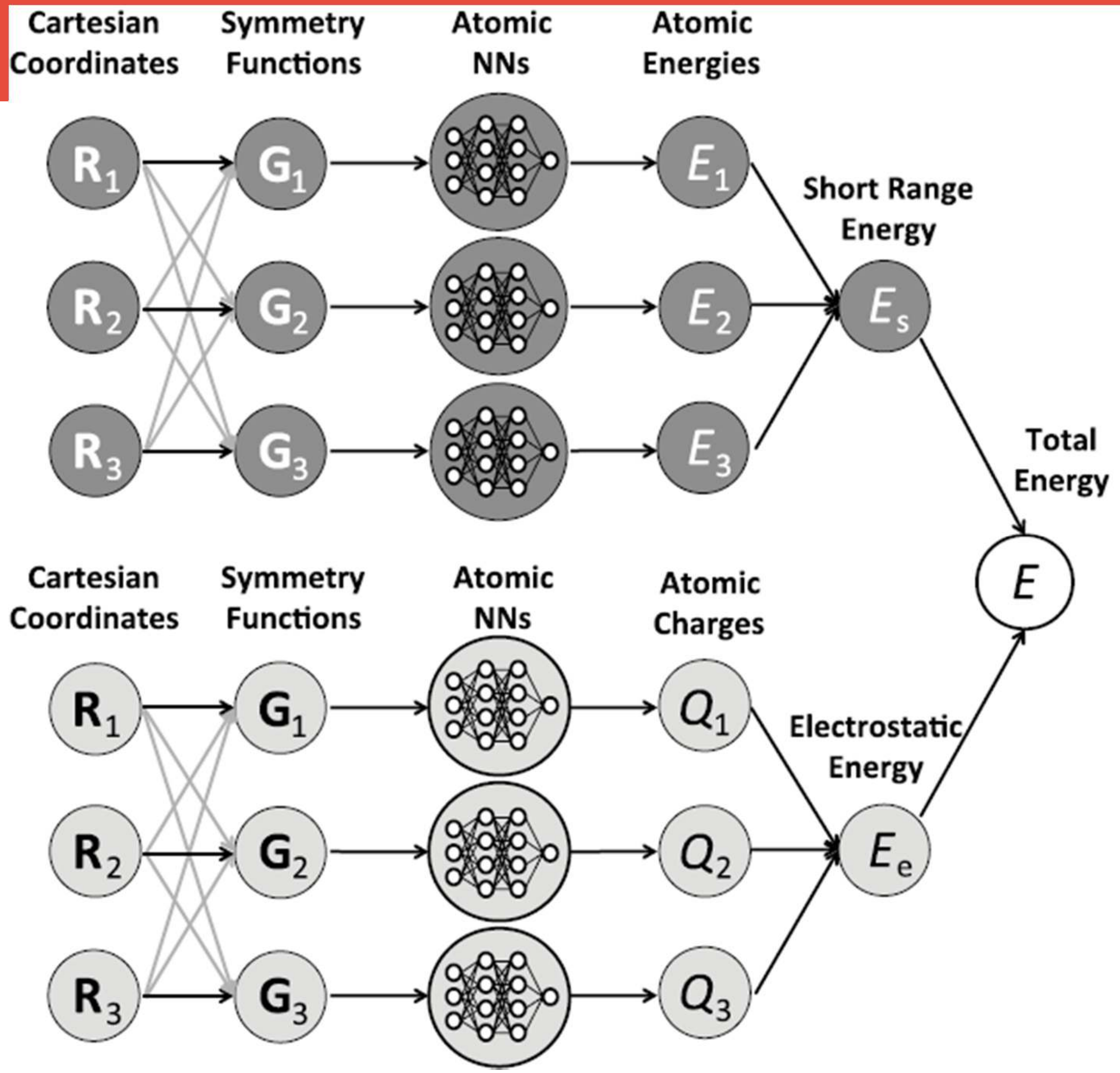


Analysis of the symmetry functions of a set of 1000 representative Lennard-Jones trimmers.

Thank you for your attention

$$e^{-\eta\left(R_{ij}^2+R_{ik}^2+R_{jk}^2\right)} \cdot f_c\left(R_{ij}\right) \cdot f_c\left(R_{ik}\right) \cdot f_c\left(R_{jk}\right)$$





Cartesian Coordinates
Symmetry Functions
Atomic NNs
Atomic Energies
R1
R2
R3
G1
G2
G3
E1
E2
E3
Short Range Energy
Es
Total Energy
E
Cartesian Coordinates
Symmetry Functions
Atomic NNs
Atomic Charges
R1
R2
R3
G1
G2
G3
Q1
Q2
Q3
Electrostatic Energy
Ee