ACCURATE DEEP NEURAL NETWORK POTENTIAL FOR PREDICTING PROPERTIES OF SOLIDS

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Machine learning and Artificial Neural Networks. What and why?

Artificial Neural Network for description of the interatomic potential

What it can do?
ML Applications
Scheme of the perceptron

\[ f(\sum_{i=1}^{n} W_i X_i) \]

- X1
- X2
- X3

W1
W2
W3

Y

Neural network diagram
Descriptors

Representation of a crystal structure in a way suitable for the NN

Invariant with respect to:

- Translation and rotation
- Atom indexing
- System size and composition
HOW IT WORKS?

\[ r_{K_iK_j} \Rightarrow f \left( r_{K_iK_j} \right) \]

\[ f \left( r_{K_iK_j} \right) = e^{-\sigma \left( r_{K_iK_j} - \eta \right)^2} \]

\[ Z_{K_i} \Rightarrow c_{K_i} \]

\[ D_i^l = \sum_j c_{K_i}^l c_{K_j}^l e^{-\sigma \left( r_{K_iK_j} - \eta \right)^2} f_c \left( r_{K_iK_j}, R_c \right) \]

\[ E_{tot} = \sum_{i=1}^{N} E_{K_i} \]

\[ J = \sum_i \left( E_{tot} - E_{DFT} \right)^2 + \lambda \sum_i \left( F - F_{DFT} \right)^2 \]

\[ F = -\frac{dE_{tot}}{dx} \]
Accuracy

- Energy: ~ 1 meV/atom
- Forces: 0.003 – 0.05 eV/Å

Features

- Output: Energy, Forces, Stress tensor
- Efficient training utilizes both energies and forces
- Training data may contain any number of atoms and species
Phases of SrTiO$_3$

High T phase

Low T phase

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<th>Wave vector</th>
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WHAT IT CAN DO?

Anharmonicity

**300 K**

- **108 atoms**
- **775 K**
- **2048 atoms**
- **10976 atoms**
CONCLUSIONS

Benefits

- Universality
- Accuracy
- Efficiency

Problems

- Data for training
- Black box style