DE LA RECHERCHE À L'INDUSTRIE

ACCURATE DEEP NEURAL NETWORK POTENTIAL FOR PREDICTING PROPERTIES OF SOLIDS

ICMPE | Bochkarev Anton

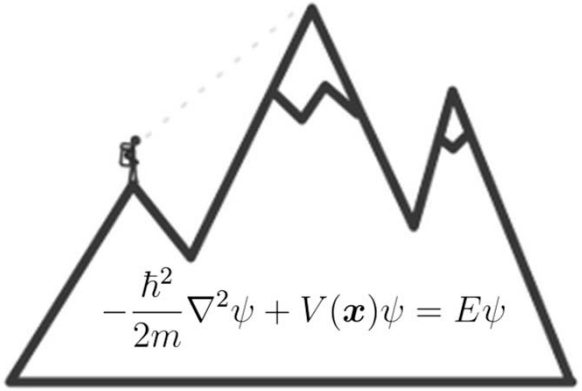
Natalio Mingo, Ambroise van Roekeghem, Stefano Mossa
CEA, Grenoble

25 SEPTEMBER 2018

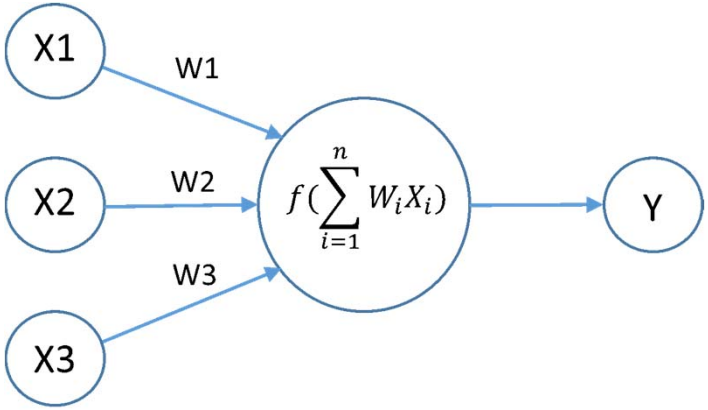
OUTLOOK

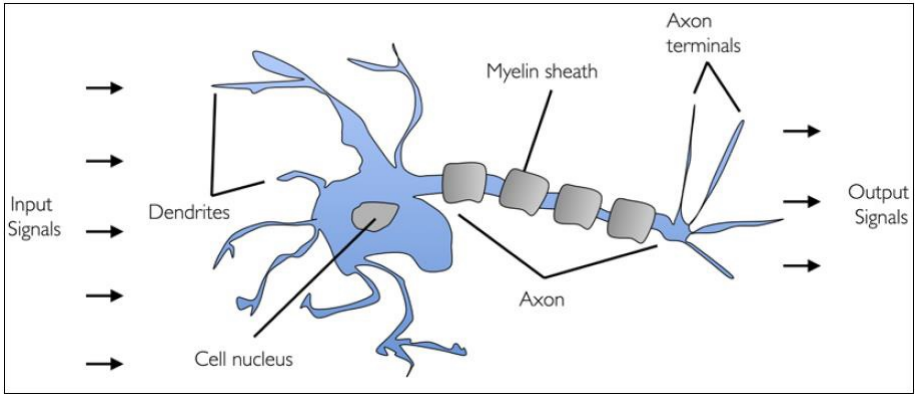
- Machine learning and Artificial Neural Networks. What and why?
- Artificial Neural Network for description of the interatomic potential
- What it can do?

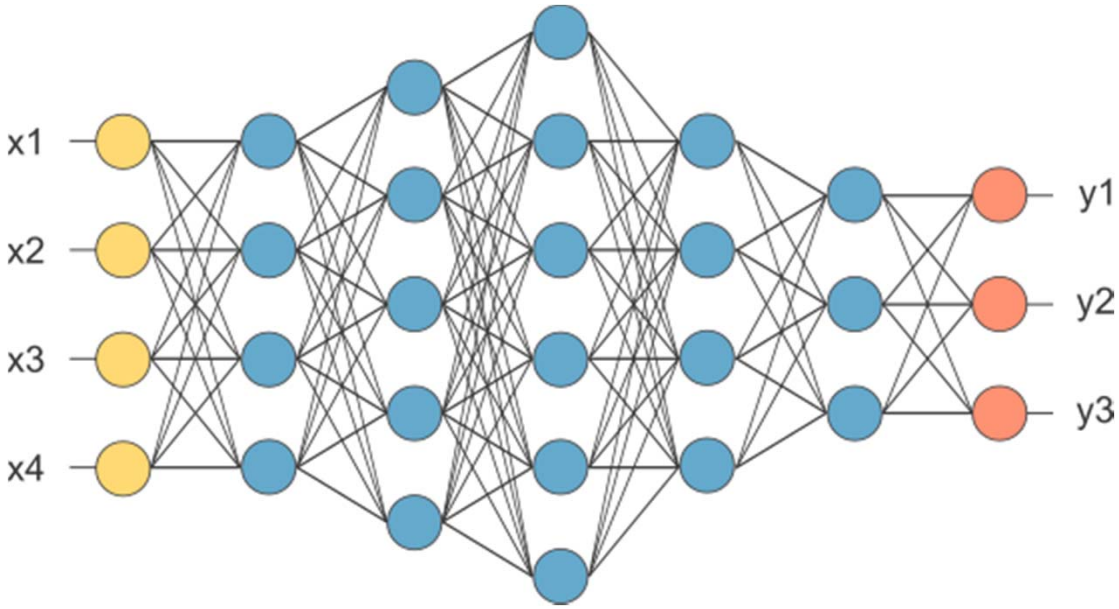
ML Applications



Scheme of the perceptron







Descriptors

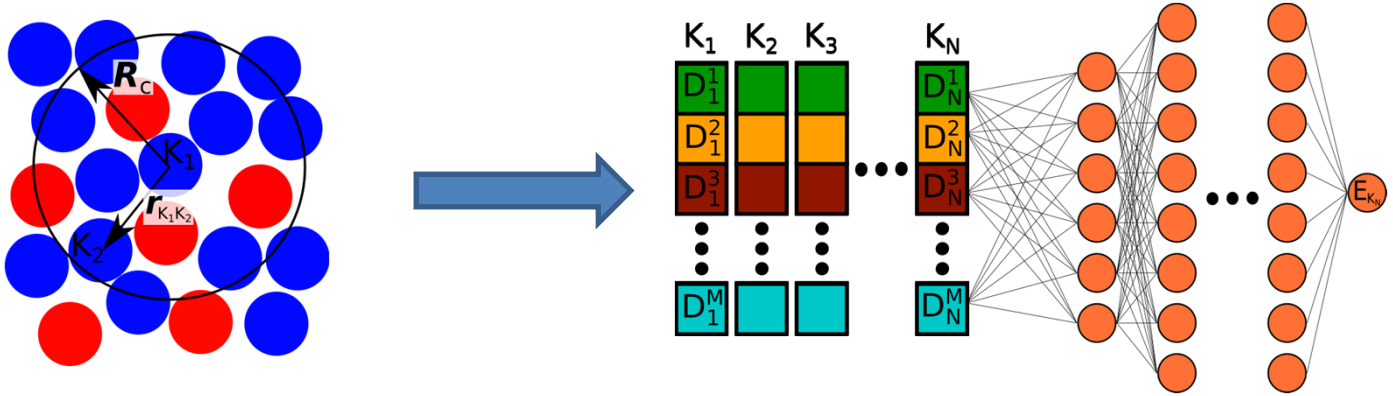
Representation of a crystal structure in a way suitable for the NN

Invariant with respect to:

- Translation and rotation
- Atom indexing
- System size and composition

J. Chem. Phys. 145, 170901

HOW IT WORKS?



$$r_{K_iK_j} \Rightarrow f\left(r_{K_iK_j}\right)$$

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

$$Z_{K_i} \Rightarrow c_{K_i}$$

$$D_i^l = \sum_{j}^{r_{K_iK_j}<R_c} c_{K_i}^l\, c_{K_j}^l\, e^{-\sigma^l\left(r_{K_iK_j}-\eta^l\right)^2} f_c\left(r_{K_iK_j}, R_c\right)$$

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

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

$$F \quad = -\frac{dE_{tot}}{dx}$$

CHARACTERISTICS OF THE POTENTIAL

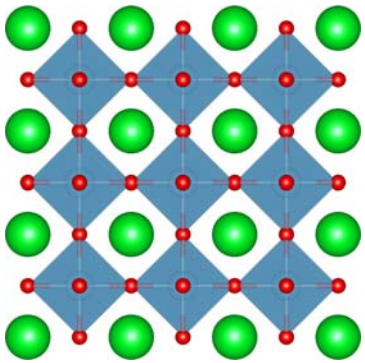
Accuracy

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

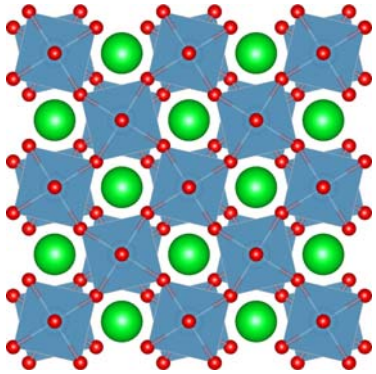
Features

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

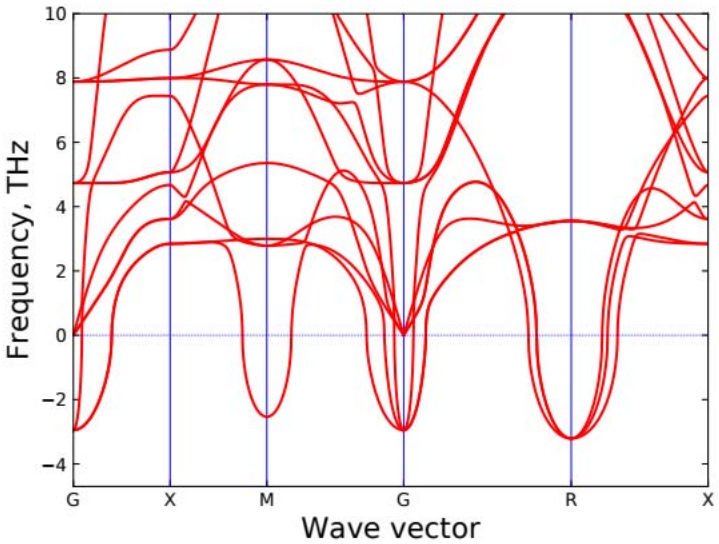
Phases of $SrTiO_3$

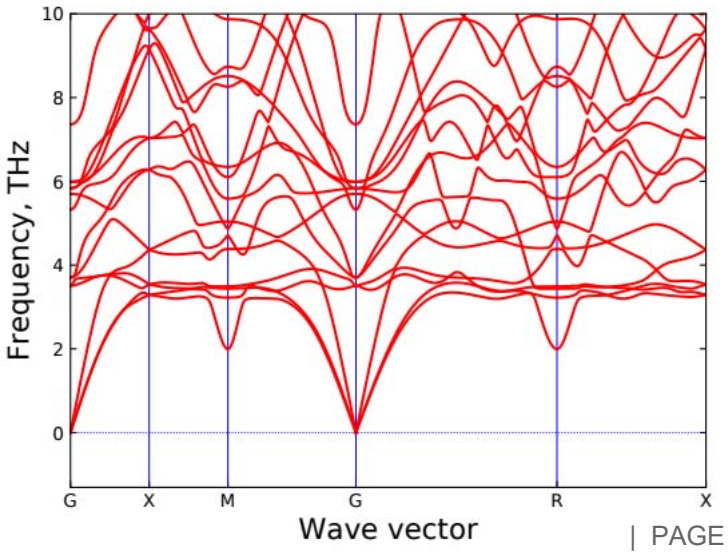


High T phase

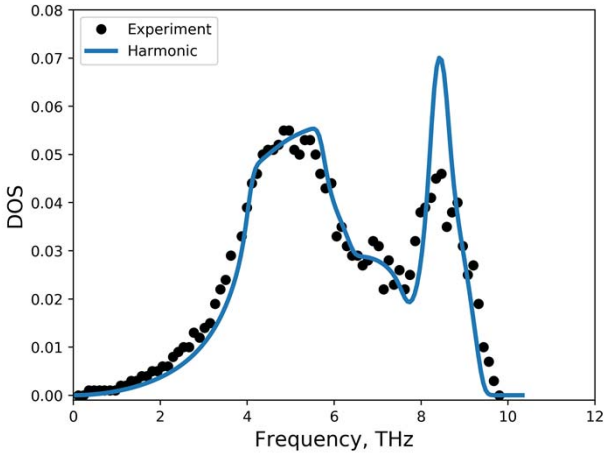


Low T phase

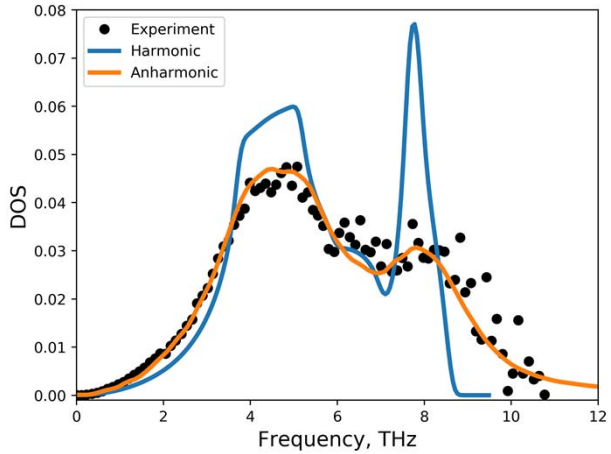




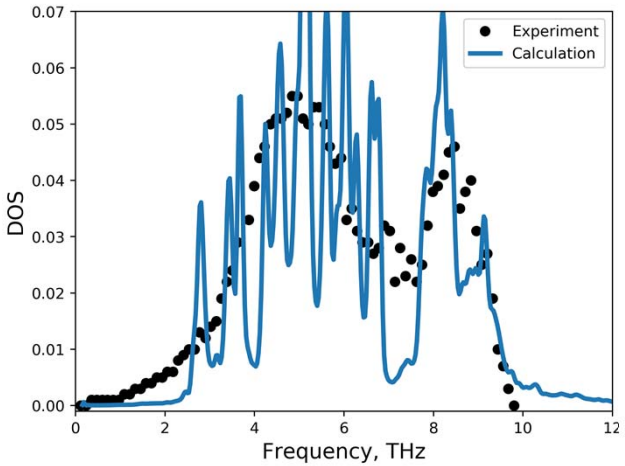
Anharmonicity



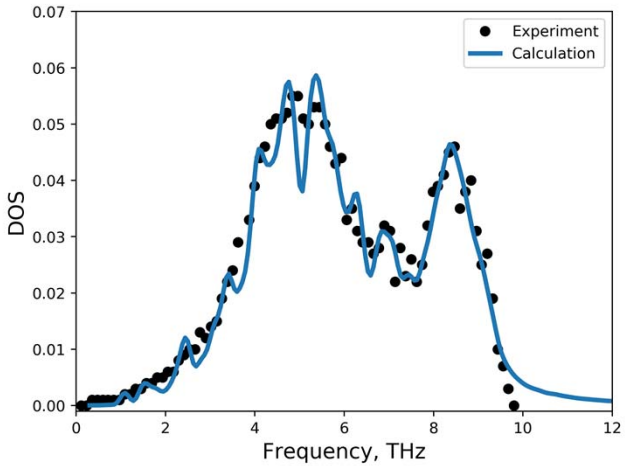
300 K



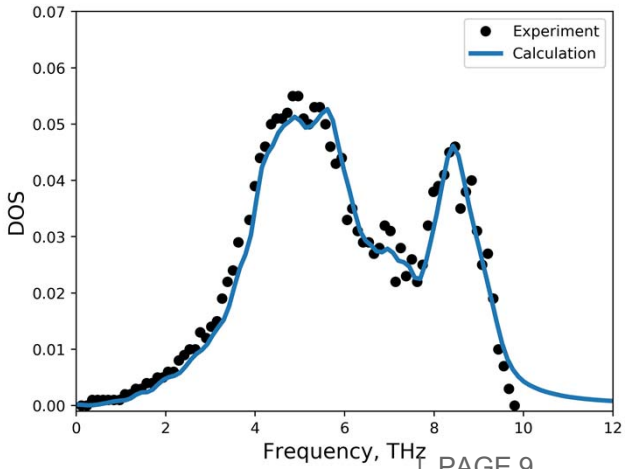
775 K



108 atoms



2048 atoms

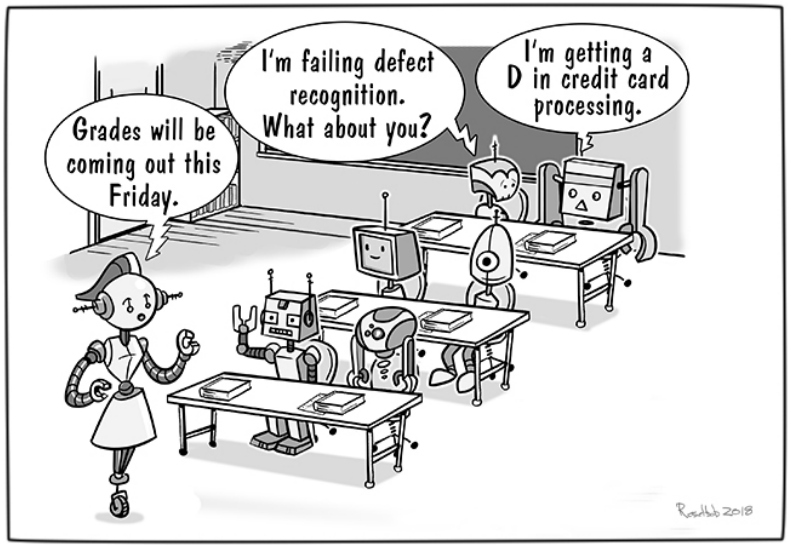


10976 atoms

CONCLUSIONS

Benefits

- Universality
- Accuracy
- Efficiency

Problems

- Data for training
- Black box style