Skoltech & MIT Conference
"Shaping the Future: Big Data, Biomedicine and Frontier Technologies"
Skolkovo Innovation Center, Moscow, April 25th-26th, 2017

MACHINE LEARNING FOR CRYSTAL STRUCTURE PREDICTION

Evgeny Podryabinkin[1], Evgeny Tikhonov[2,3],
Alexander Shapeev[1], Artem R. Oganov[1,3]

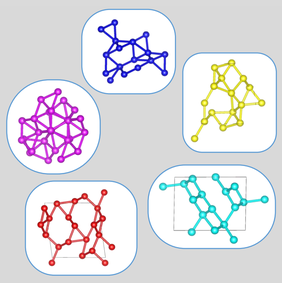
[1] Skolkovo Institute of Science and Technology,
[2] M.V.Lomonosov Moscow State University
[3] Moscow Institute of Physics and Technology.

Crystal Structure Prediction Method

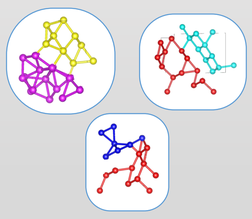
USPEX Computational Materials Discovery

USPEX is an evolutionary algorithm for crystal structure prediction. It has been used in many important material discoveries.

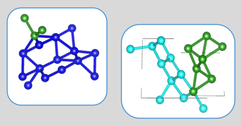
1. Initial structures
   a. Randomly generated
   b. Kept from previous generation



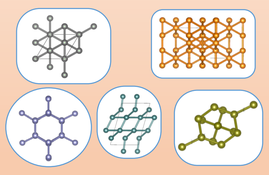
2. Transformation
   a. Cross



   b. Mutation

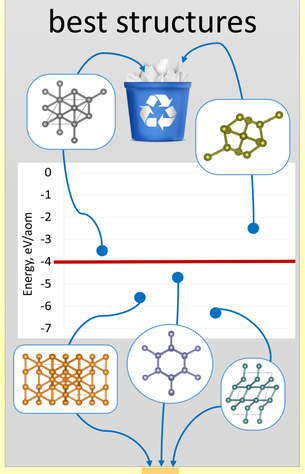


3. Relaxation with Density Functional Theory (DFT)



The most computationally expensive stage. It takes ~99.9% of CPU time

4. Sorting and selection of the best structures



Best structures produce next generation

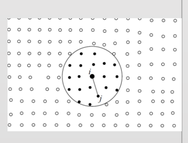
+

Machine Learning Model of Interatomic Interaction

MTP

Moment Tensor Potentials (MTPs) are a machine learning model of interatomic interaction. It can compute energy, forces, and stresses, approximating a given quantum-mechanical (QM) model. MTPs are successfully used for many applications of atomistic modeling.

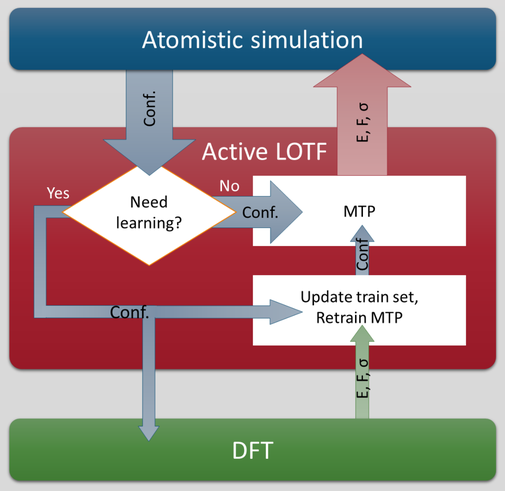
Features of MTPs:



- MTPs are local, i.e., energy of each atom depends on positions of neighboring atoms within a cutoff sphere.
- This dependence is invariant w.r.t. rotations and permutations of atoms of the same type.
- MTPs have a number of a priori unknown parameters found by requiring that the total energy, forces on atoms and stresses are close to their QM counterparts on the training set.
- Linear regression for finding parameters is employed.
- MTP is able to approximate any QM model with an arbitrary accuracy (at least theoretically) by increasing the number of parameters.
- MTP scales linearly with the number of atoms.

Learning on the fly

- Active learning allows an MTP to select important configurations for fitting, thus constructing a training set.
- Active learning enables learning on the fly (LOTF, see the scheme bellow).



—

Advanced method for novel materials discovery

We have implemented MTPs for USPEX.
MTP have replaces much more expensive DFT for structure relaxation and energy evaluation. This yields a significant (orders of magnitude) acceleration.

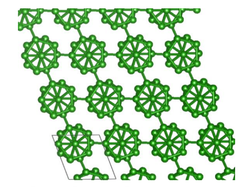
Testing

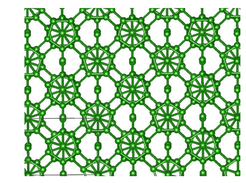
- Testing on Carbon and Boron structures.
- Boron is a good choice for thorough testing:
  - A lot of allotropes (hard to find the best ones among the enormous number of the suboptimal ones).
  - Small energy difference among allotropes (requires very accurate energy approximation).
  - Some allotropes have more than 100 atoms.
- MTP has been trained on the fly.
- Some of the low-energy Boron structures found with MTP are shown in the right section.

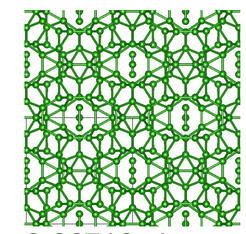
Summary

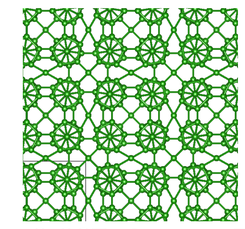
- Machine learning model of interatomic interaction has been applied to crystal structure prediction, replacing expensive DFT.
- This yields acceleration by orders of magnitude.
- This also enables finding the structures with a large number of atoms in the supercell (up to 100+ atoms), which was not possible before.

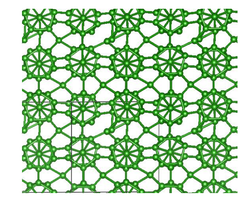
Some of the best (low energy) Boron allotropes found by USPEX with MTP. Structures provided with energy per atom, number of atoms in the unit cell and typical time to find (on 16 CPU cores)

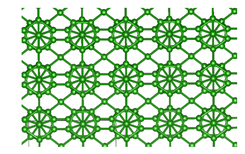

E=-6.70578, Atoms: 12
1 hour vs. 1 week with DFT

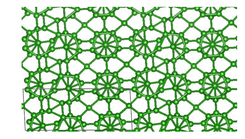

E=-6.6782, Atoms: 28
2 days vs. 1 month with DFT

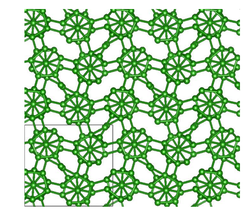

E=-6.66712, Atoms: 54
4 days vs. 2 years with DFT

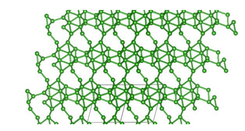

E=-6.667, Atoms: 52
4 days vs. 2 years with DFT

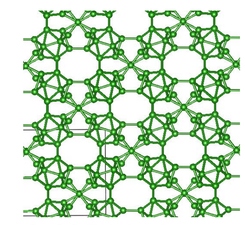

E=-6.6667, Atoms: 106
2 weeks with MTP

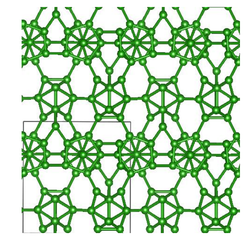

E=-6.6649, Atoms: 26
1 day vs. 1 month with DFT

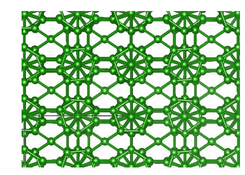

E=-6.6497, Atoms: 36
2 days vs. 3 months with DFT

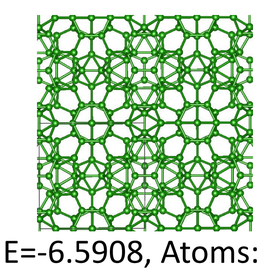

E=-6.6493, Atoms: 52
4 weeks vs. 1 year with DFT


E=-6.6327, Atoms: 20
12 hours vs. 2 weeks with DFT


E=-6.62514, Atoms: 60
6 days vs. 2 years with DFT


E =-6.6174, Atoms: 50
3 days vs. 10 months with DFT


E =-6.6037, Atoms: 100
1.5 weeks with MTP


E=-6.5908, Atoms: 108
2 weeks with MTP