Machine learning for Materials Research

DJURABEKOVA FLYURA

HELSINKI INSTITUTE OF PHYSICS AND DEPARTMENT OF PHYSICS

UNIVERSITY OF HELSINKI

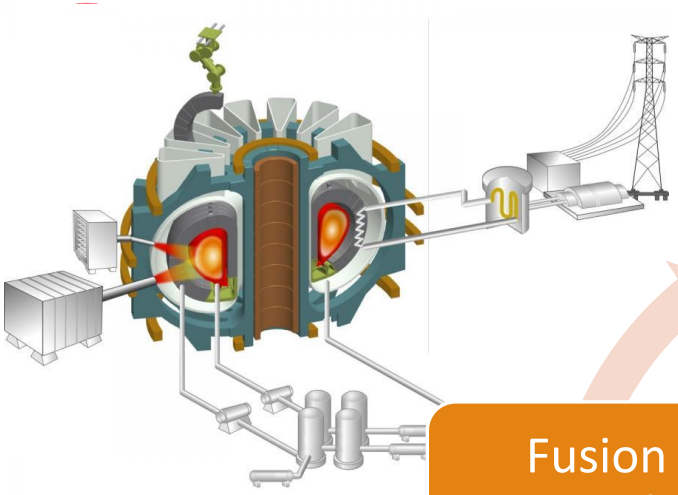
FINLAND

Collaborators and colleagues

- Reactor Materials Research UNIT, SCK•CEN, MOL, BELGIUM
  - Domingos R.
  - Castin N.c
  - Malerba L.
  - Cerchiara G.
- University of Helsinki
  - Jyri Lahtinen
  - Ville Jansson
  - Ekaterina Baibuz
  - Kai Nordlund

Source of energy = source for life

Humanity keeps searching for affordable sources of energy.



Bonfire

Fireplace

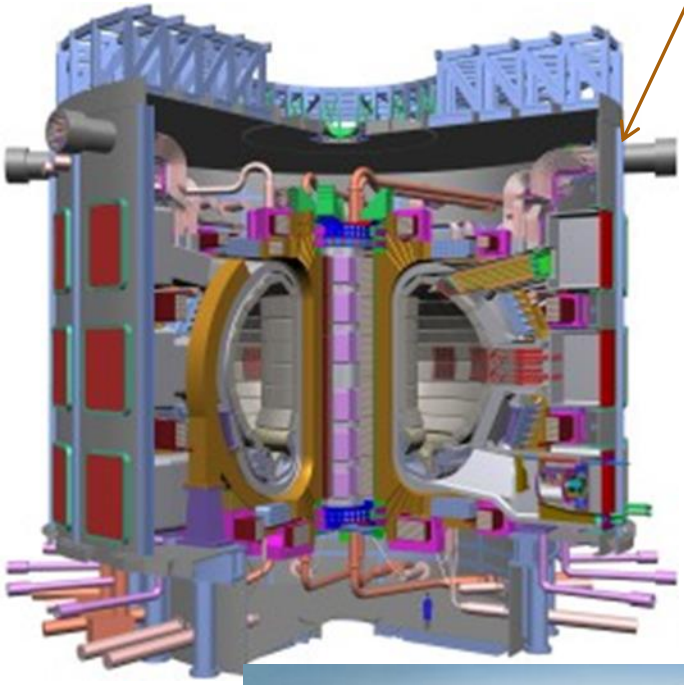
Coal power plant

Nuclear power plant

Fusion power plant

Efficient generation of energy requires new construction materials

ITER



Nuclear power plant

By Emmelie Callewaert - Own work, CC BY-SA 4.0, https://commons.wikimedia.org/w/index.php?curid=36226832

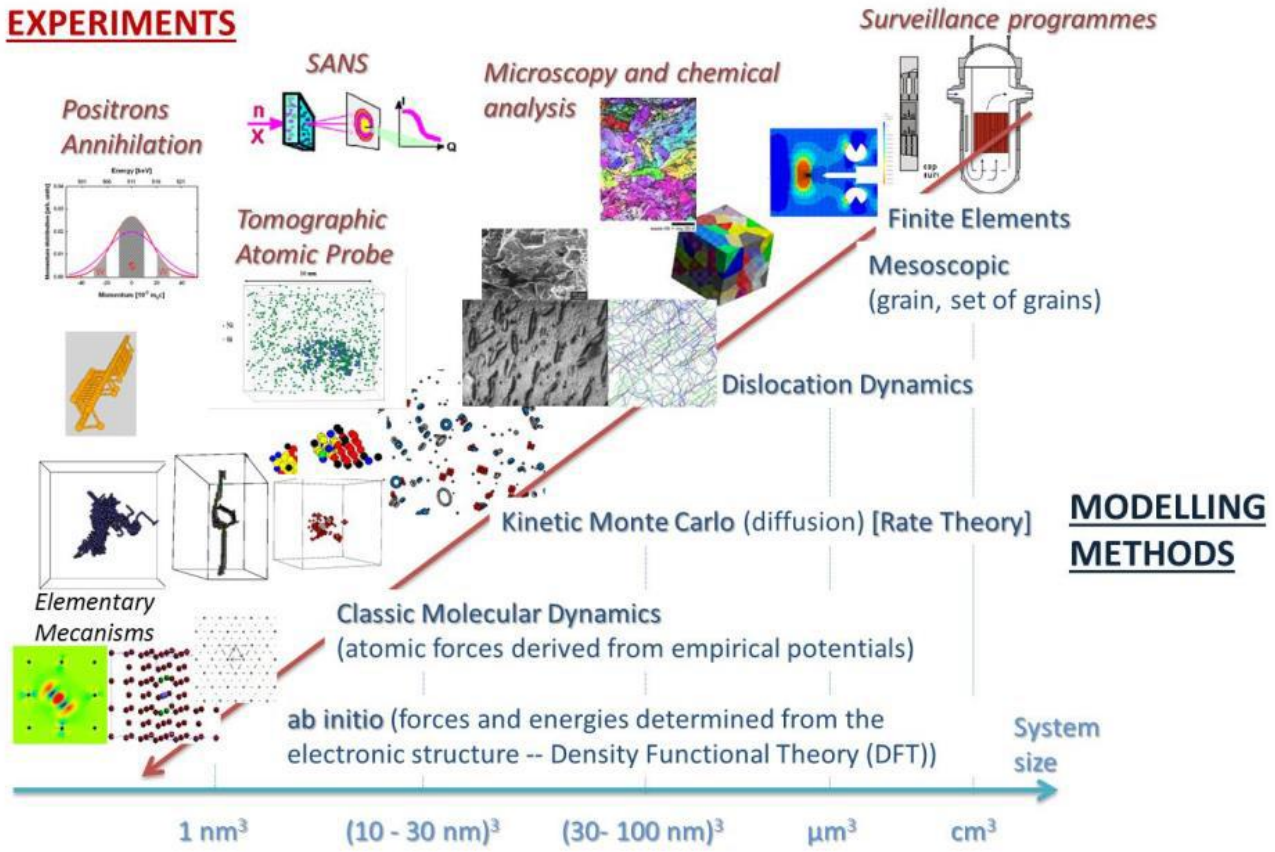
Future particle collider

Reactor pressure vessel

Many of the Generation II reactors were built in 1965–1980 and have now reached, or are approaching, the end of the designed life-time, which is normally 40 years.

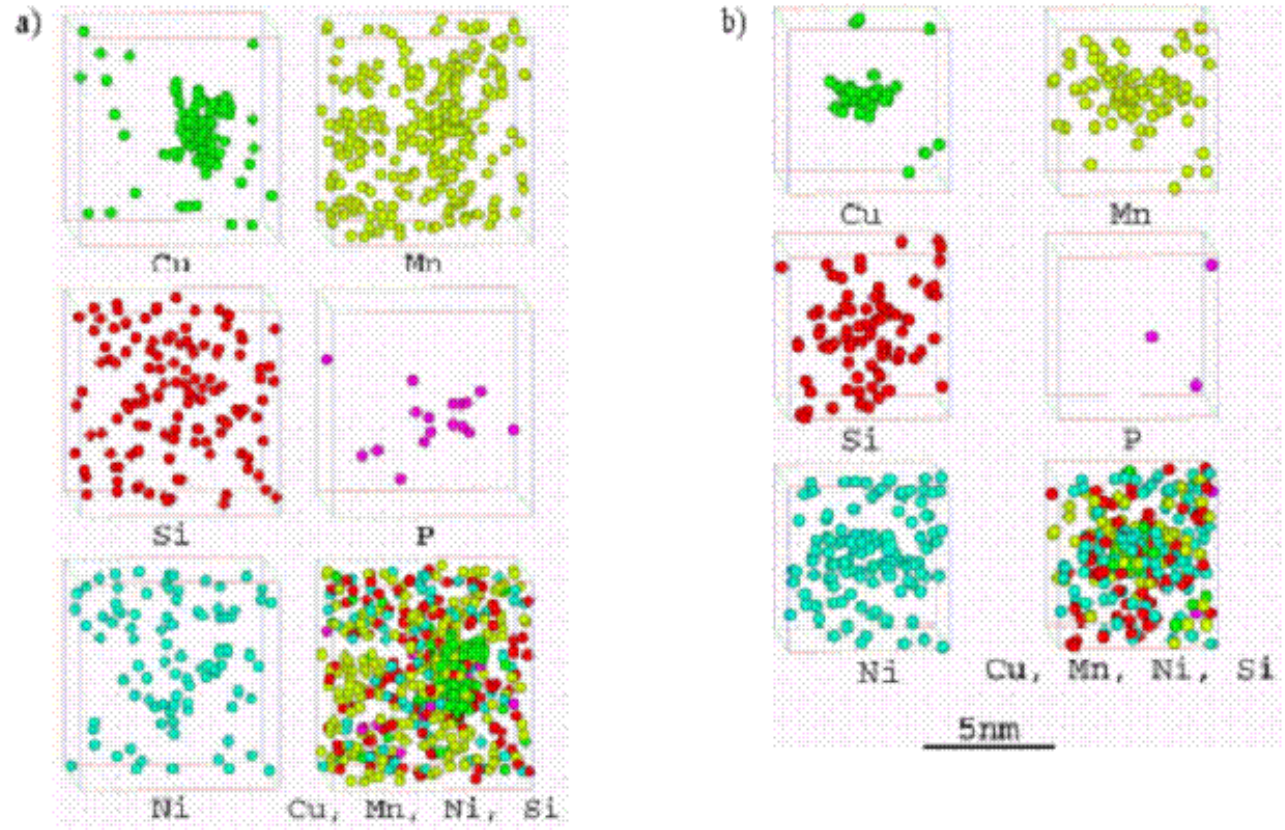
Neutron irradiation during the operation of the nuclear power plant induces defects in the steels of the reactor and cause their hardening and embrittlement. Especially the reactor pressure vessel (RPV), that contains the fuel assemblies, is vulnerable to degradation, The life-time of the RPV determines the life-time of the whole power plant.

How we develop new materials



Multi-scale approach from nano- to macro-scales: strong link between the developed modelling tools and experimental characterization techniques

Main effects of irradiation in Reactor Pressure Vessel steels - Microstructure



Experimental determination of precipitate composition in industrial ferritic steels under irradiation (3-D Atom Probe) – See P. Auger et al. J. Nucl. Mater. 280 (2000) 331 for review

Cu is the driving element for formation of complex, Ni & Mn-rich precipitates

These precipitates are likely to contain also vacancies, but 3DAP cannot detect them

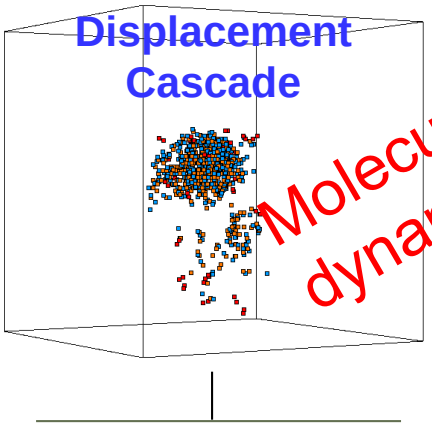
Multiscale Modelling in RPV steels

1 fs = 10^{-15} s 1-100 ps = 10^{-12}- 10^{-10} s ns = 10^{-9} s ….. ms = 10^{-3} s ….. 1 s …… 10^{3} s

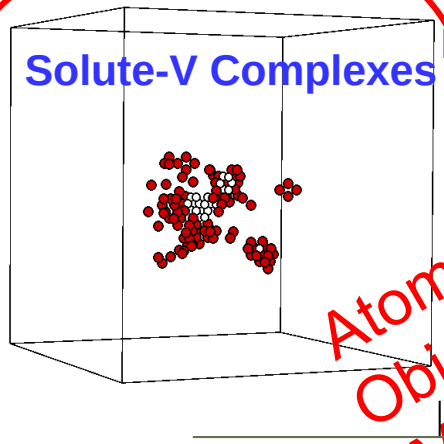
Time scale

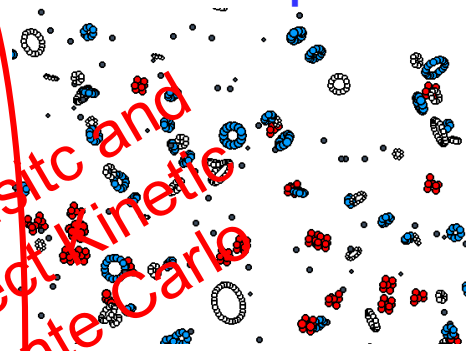
Neutron transport

From n spectrum to PKA & Displacement Cascade Spectrum



Molecular dynamics





Atomistic and Object Kinetic Monte Carlo

Collisions

Recombinations

Relaxation

Defect Migration

Secondary Defect Formation

Nucleation & Growth of Precipitates & Large Clusters

Length scale

10s of nm = 10^{-8} m 100s of nm = 10^{-7} m

Diffusion by computational Materials Science methods

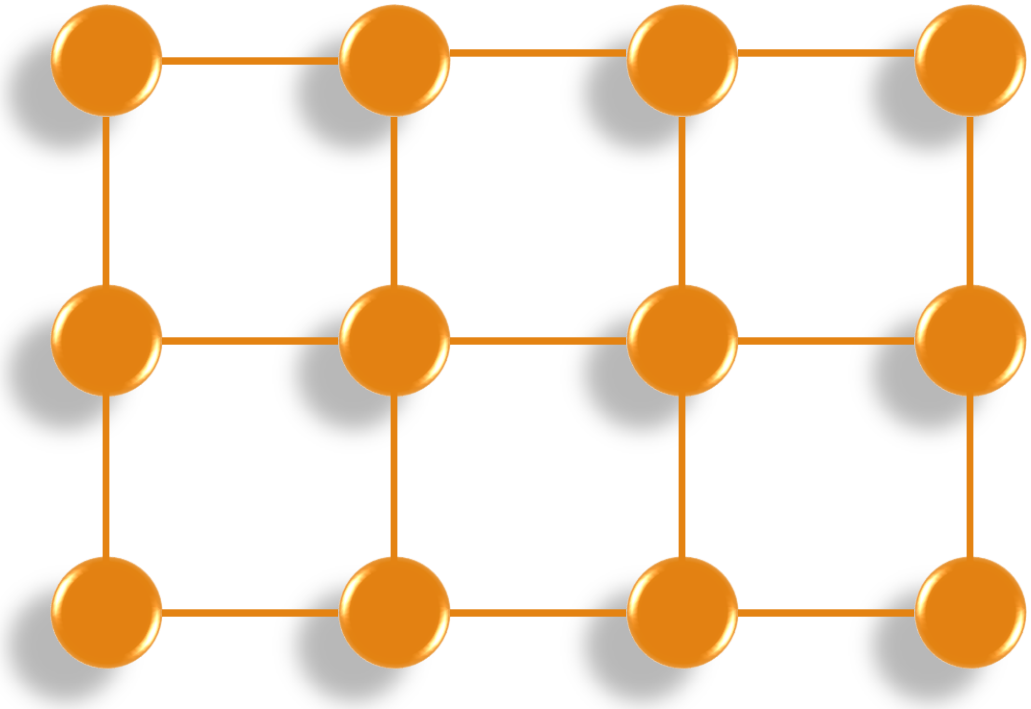
The best way to know what happens in materials after long time of operation is to consider a diffusion process of atoms.

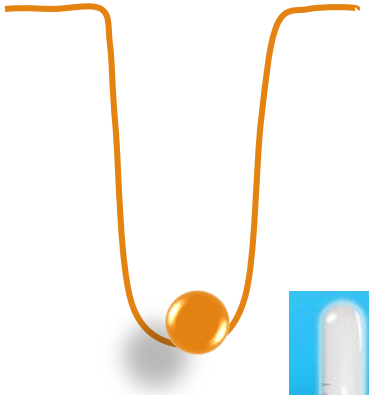
This is a very old and well known process and there numerous ways to approach this problem, for instance, solve differential equations for concentration of different species:

$$
\begin{cases}
\frac{dC_1}{dt} = & K^{21}\cdot C_2 + K^{31}\cdot C_3 + K^{51}\cdot C_5 \\
& -(K^{12}+K^{13}+K^{15})\cdot C_1 \\
\frac{dC_2}{dt} = & K^{12}\cdot C_1 + K^{42}\cdot C_4 - (K^{21}+K^{24})\cdot C_2 \\
\frac{dC_3}{dt} = & K^{13}\cdot C_1 + K^{43}\cdot C_4 - (K^{31}+K^{34}+K^{3\infty})\cdot C_3 \\
\frac{dC_4}{dt} = & K^{24}\cdot C_2 + K^{34}\cdot C_3 + K^{54}\cdot C_5 \\
& -(K^{42}+K^{43}+K^{45}+K^{4\infty})\cdot C_4 \\
\frac{dC_5}{dt} = & K^{15}\cdot C_1 + K^{45}\cdot C_4 - (K^{51}+K^{54}+K^{5\infty})\cdot C_5
\end{cases}
$$

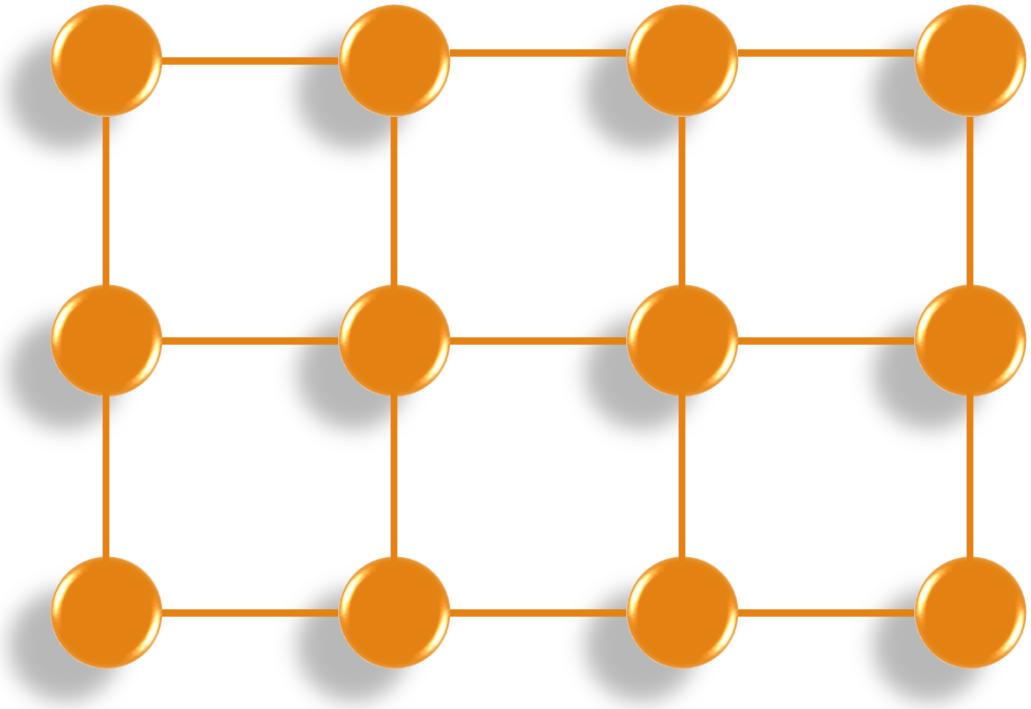
But, one can follow pretty accurately the whole kinetics of the process by setting up an algorithm of an atom jumping in the lattice

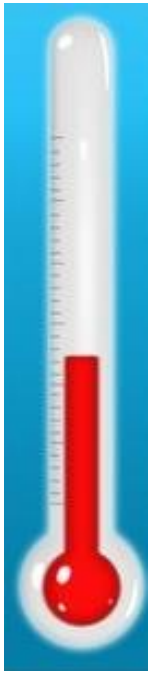
Perfect 2D metal lattice



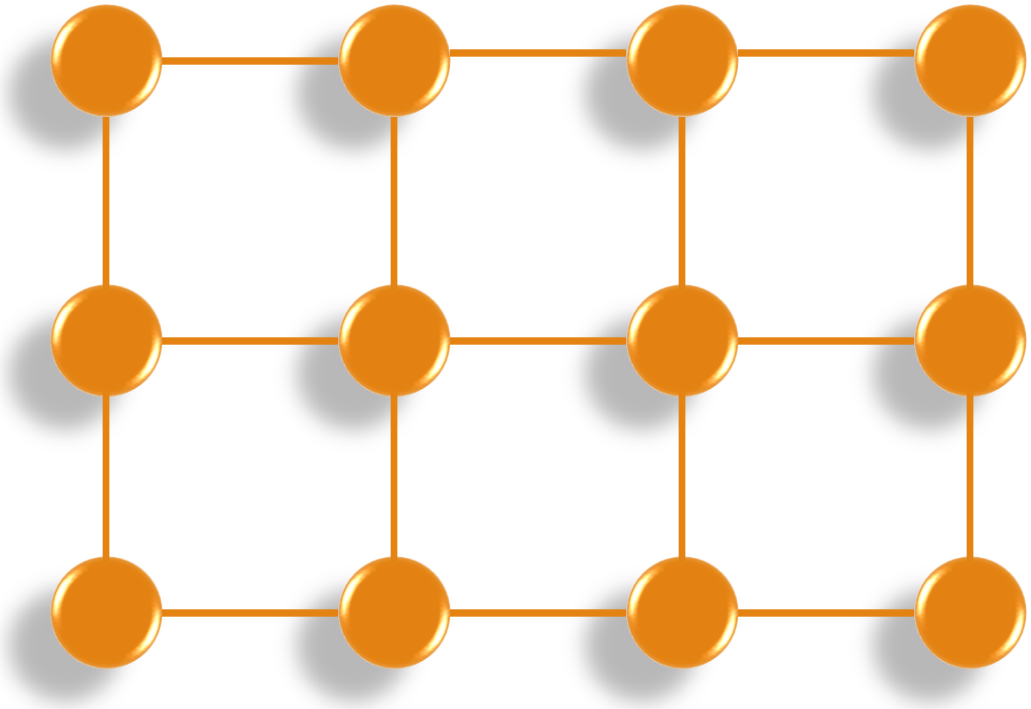


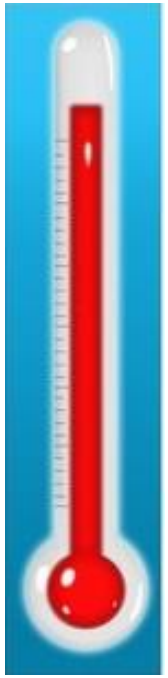
In a perfect metal crystal the atoms occupy the strictly defined positions in a lattice according to the potential of interatomic interactions.



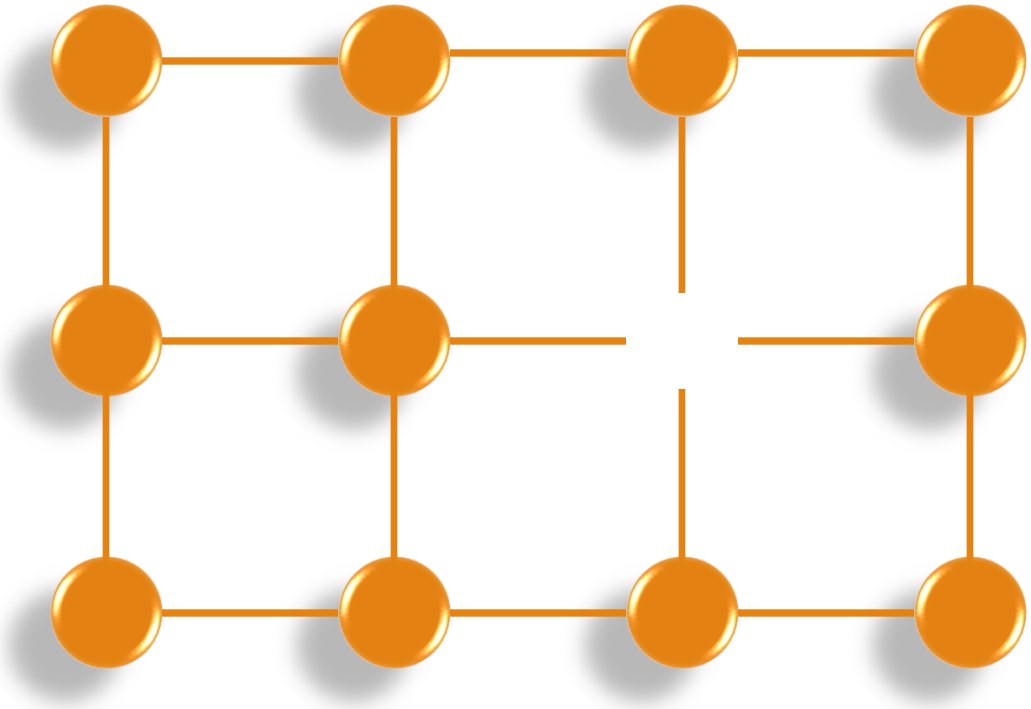


Vacancies are elemental point defects which are always present in a crystal structure



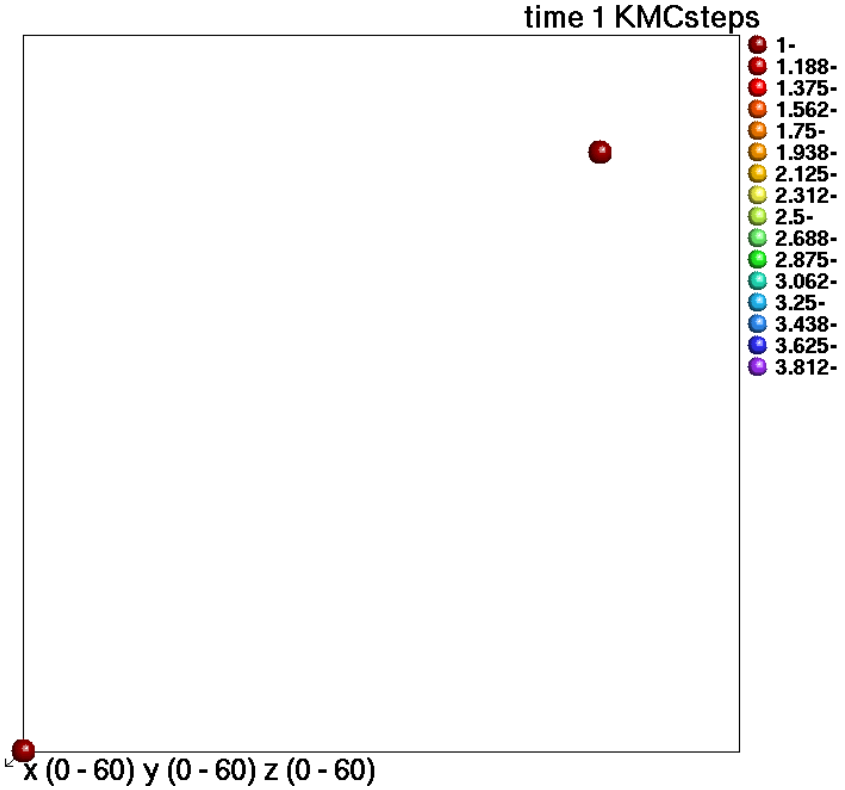


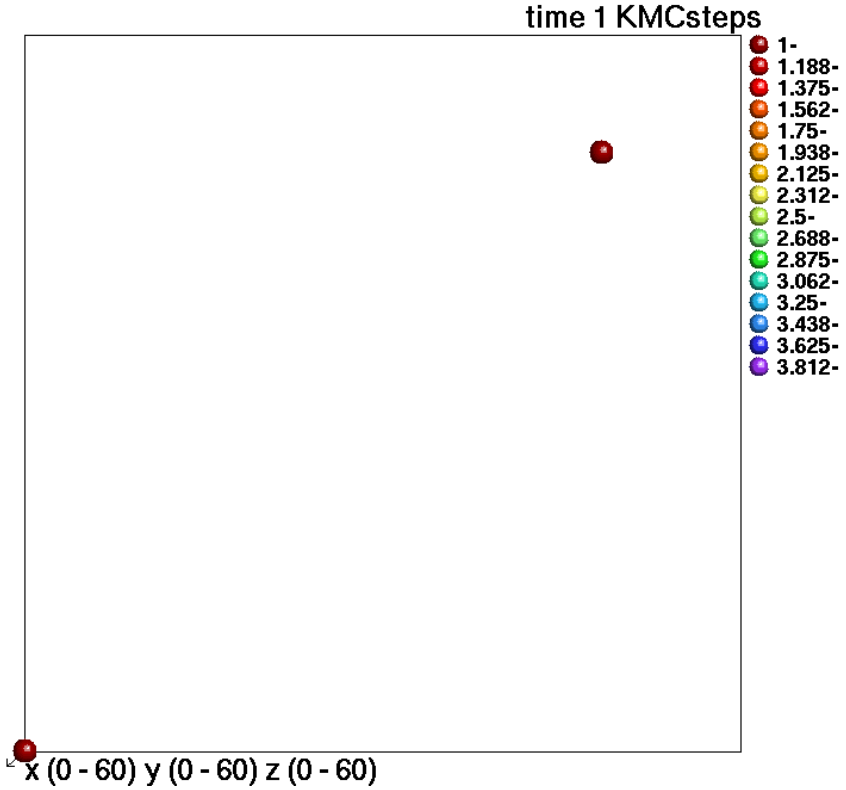
Vacancies are elemental point defects which are always present in a crystal structure



Vacancies are elemental point defects which are always present in a crystal structure

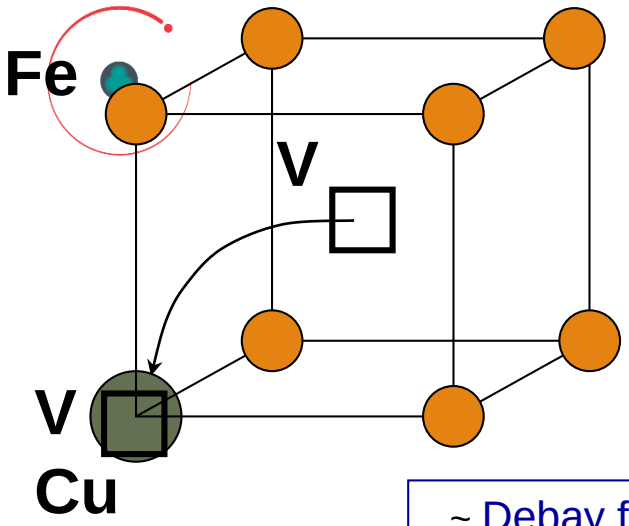
Example of 2 vacancies migrating in 3D structure





Here the red balls are vacancies, which exchange their positions with atoms (not shown in the movies)

Kinetic Monte Carlo can be used to simulate diffusion



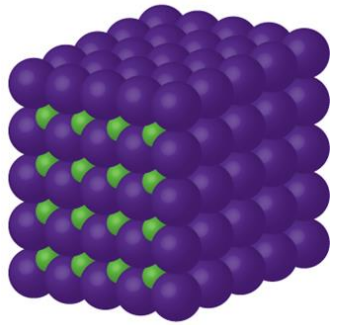
The system evolves via vacancy diffusion jumps.

The average frequency of the process, Γ, is

$$\Gamma_i = \nu_i \exp\left(-\frac{E_{a,i}}{kT}\right)$$

?

~ Debay frequency



Each jump has a probability; the jump to happen is chosen by extracting a random number

$$P_i = \frac{\Gamma_i}{\sum_{i=1}^{N} \Gamma_i}$$

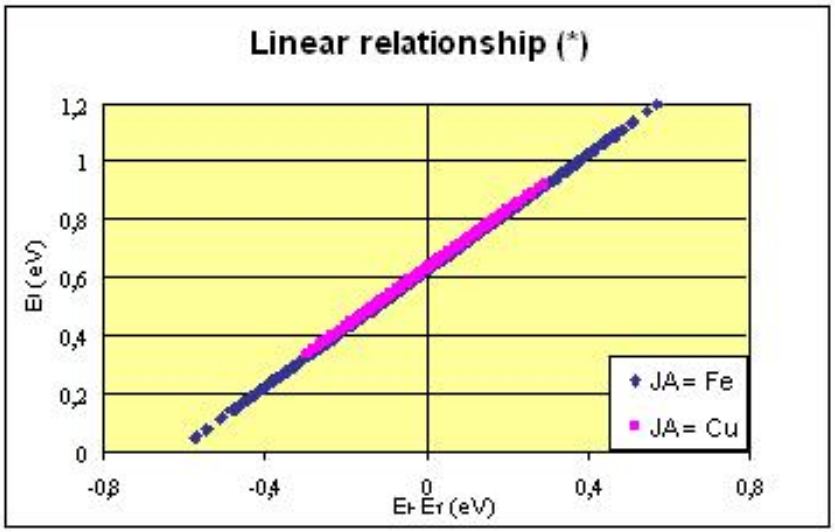
$$\sum_{i=1}^{k} P_i \le r < \sum_{i=1}^{k+1} P_i$$

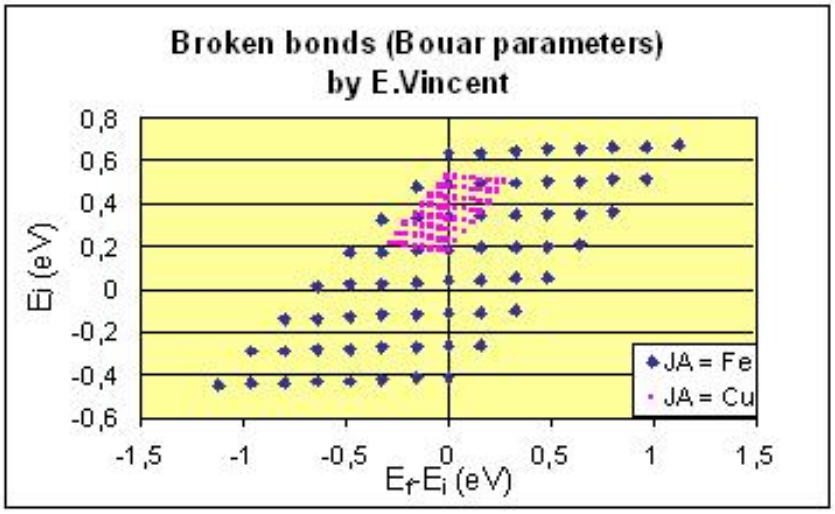
Associated time step

$$dt = \frac{-\ln(r)}{\sum_{i=1}^{N} \Gamma_i}$$

(residence time algorithm)

How to find these barriers?

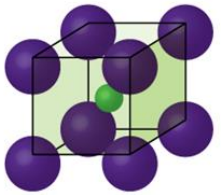




Linear relationship with energy variation

$$E_a = E_0 + \frac{E_f - E_i}{2}$$

$$E_0 = \text{constant}$$



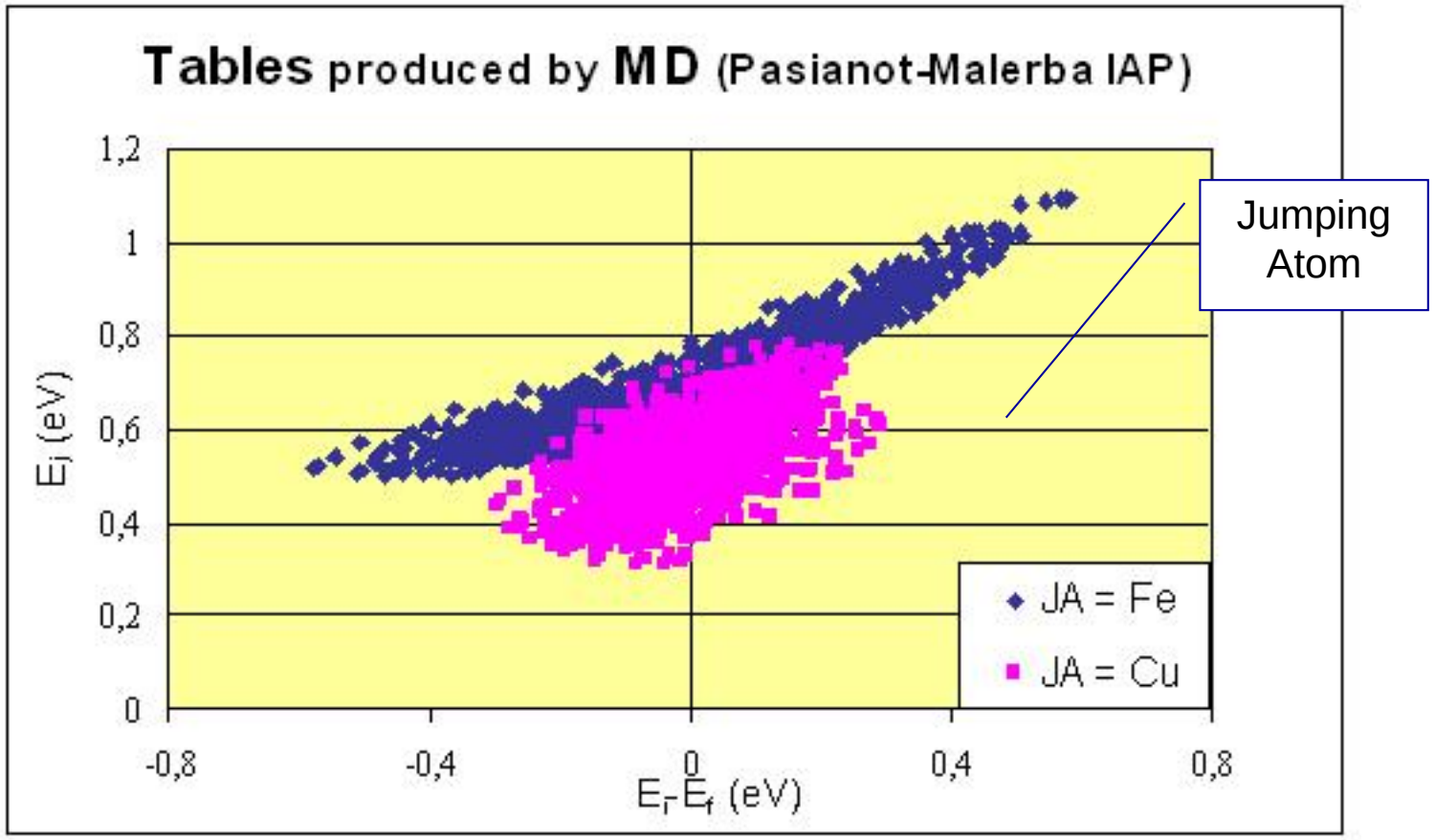
Broken bonds method

$$\Delta E^a_{i-V} = e_i^{sp} - \sum_j \varepsilon_{ij} - \sum_{j \neq i} \varepsilon_{Vj}$$

e_i^{sp} is the binding energy of atom *i* in the saddle point, summarizations correspond to the broken bonds

How these parameters look in reality

Mapping the barriers calculated by MD with an appropriate IAP versus the total energy variation shows the complexity of the relationship between the barrier and the corresponding Local Atomic Configuration (LAC)



Possible solutions

~~MD calculation at each KMC step~~

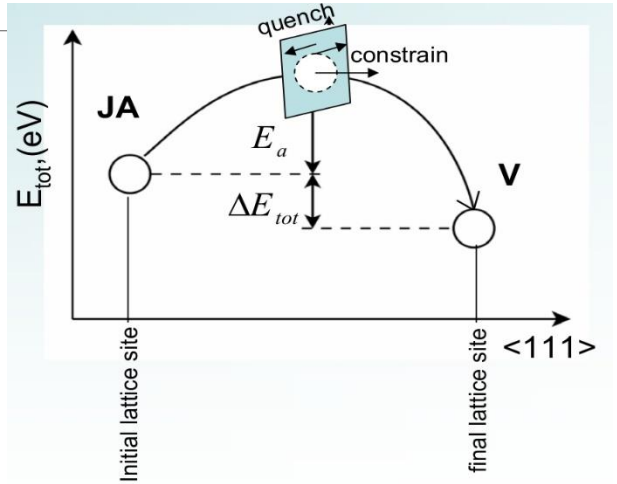
~~(takes enormous computing time)~~

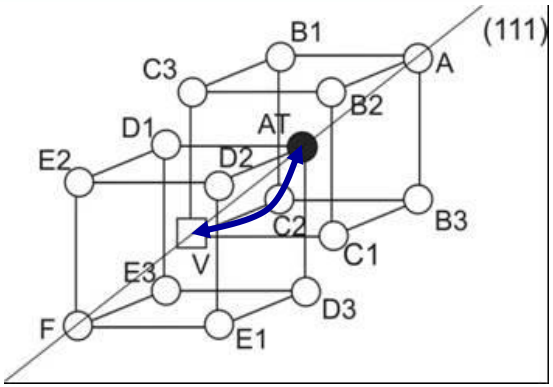
Tabulate MD calculated Ej values versus local atomic configurations, defined assigning to each lattice site A, B1, B2 etc. an integer number

Feasibility: limited number of environments is encountered in the simulation (small clusters) or only nearest neighbors are considered

Artificial intelligence assistance:

- use tables to train AI system to produce the value of the energy barrier





Example of line in the table:

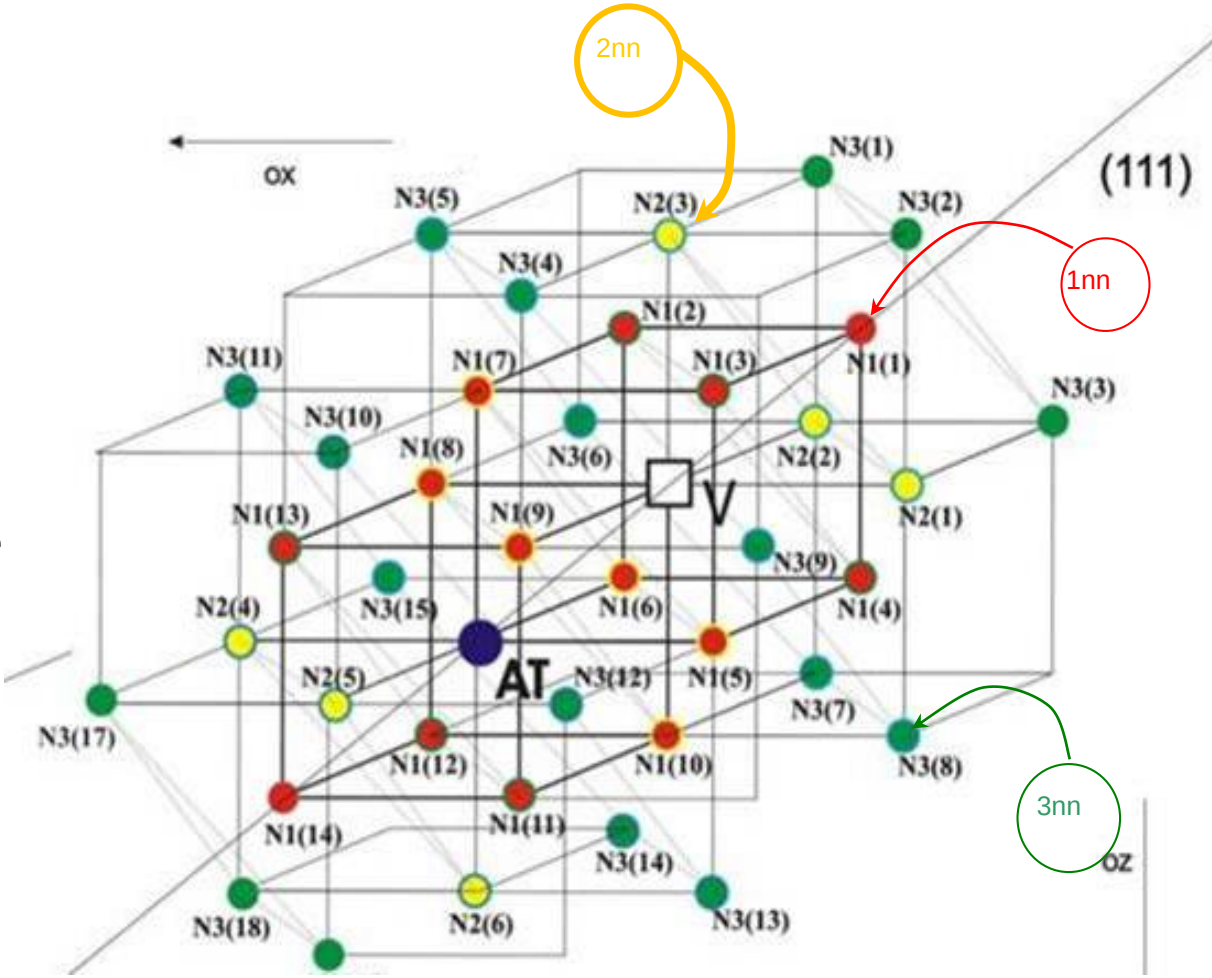
LAE	E_j
1 1 0 0 1 1 1 0 0 2 0 2 1 1 1	0.77

Local Atomic Environment

The real scale of the problem

1nn gives still manageable size of the table ($2x3^{14}$ lines)

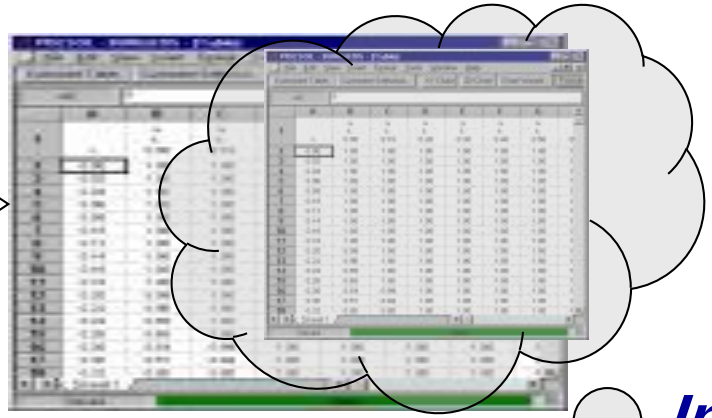
Considering all the lattice sites up to 3nn increases the number of lines to $2x3^{38}$! (~ $3x10^{18}$)



⇒ With tables it is impossible to go beyond 1nn approximation

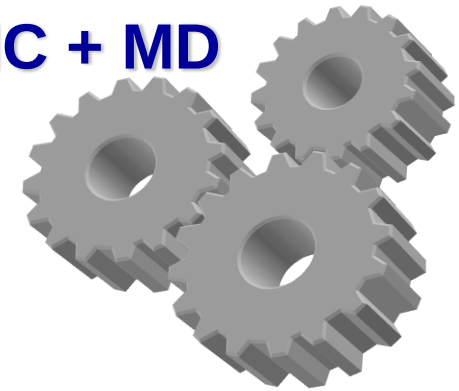
Where artificial intelligence comes into play

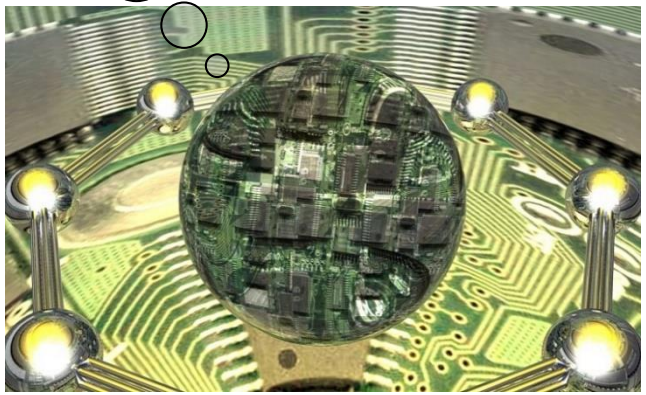
Huge table



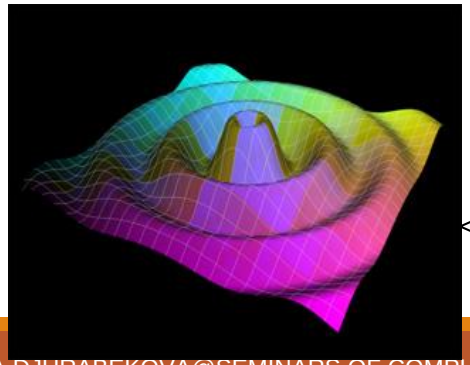
Artificial Intelligence

KMC + MD



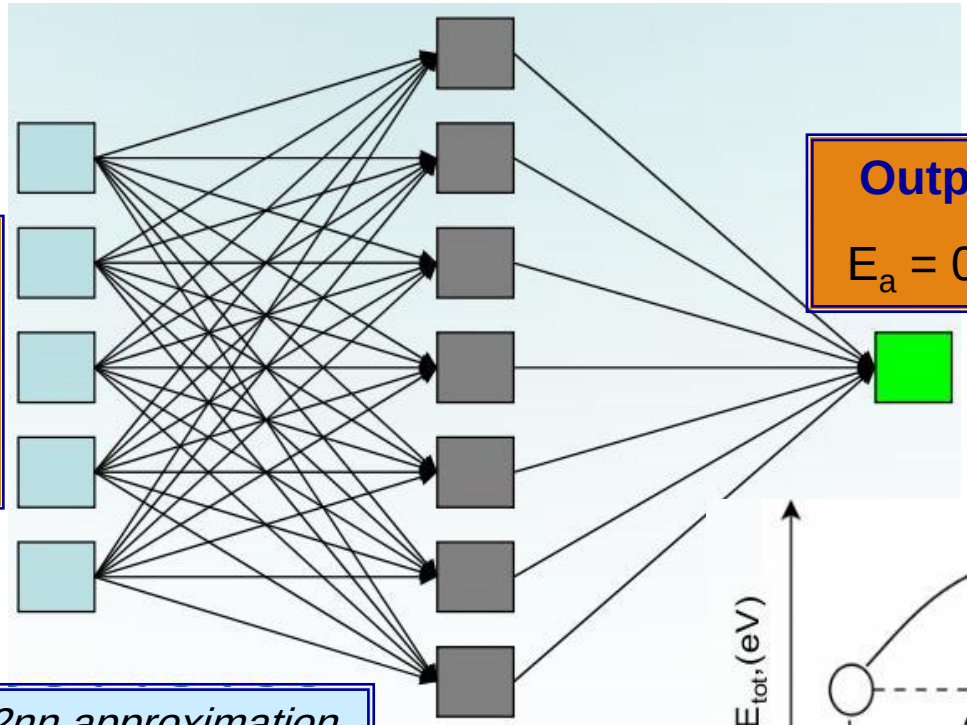


Model



Artificial Neural Network (ANN)

Multylayer perceptron with one hidden layer based on *backpropagation* learning algorithm



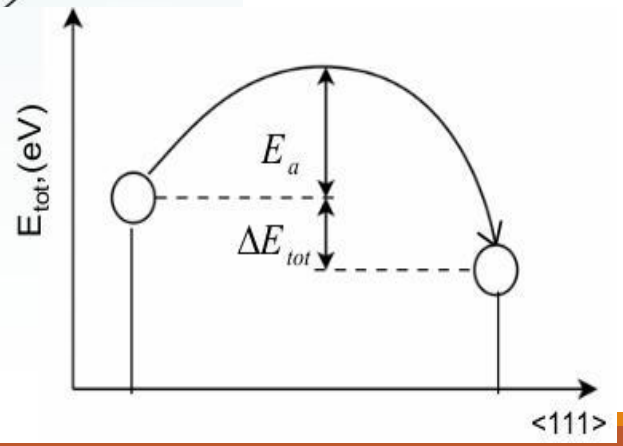
Hidden layer

Input: LAE

Line of 15 … 39 integers depending on approximation

Output:

E_a = 0,68

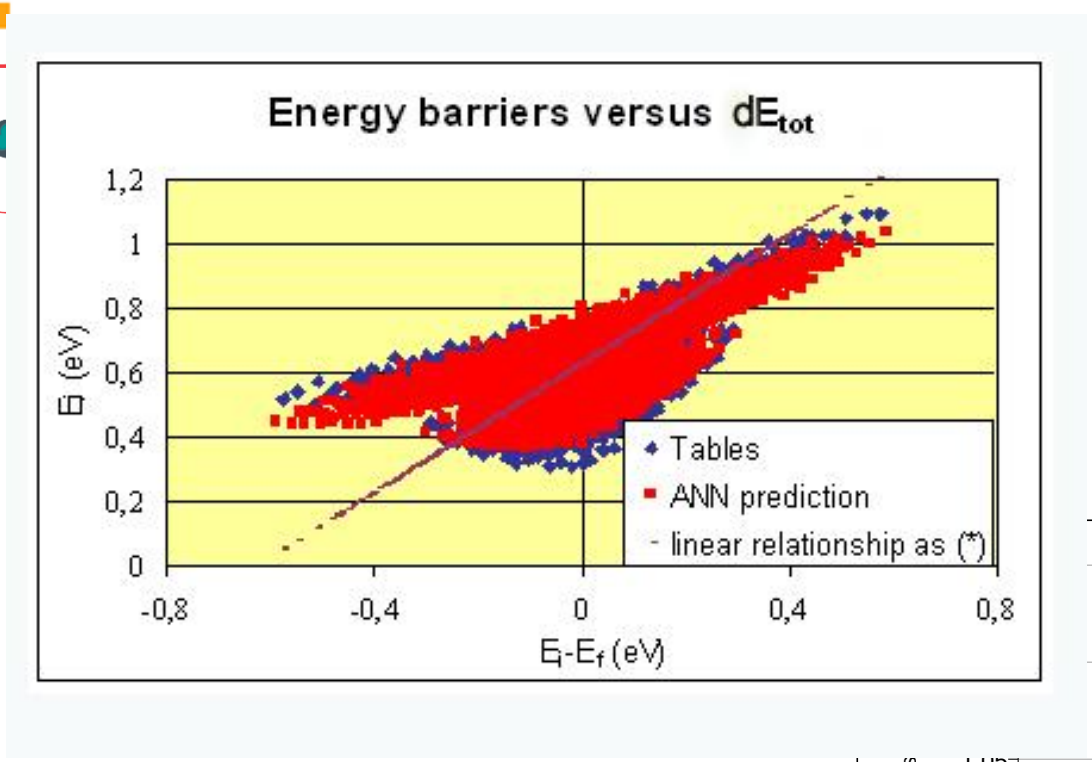


Example of **LAE** *for 2nn approximation*

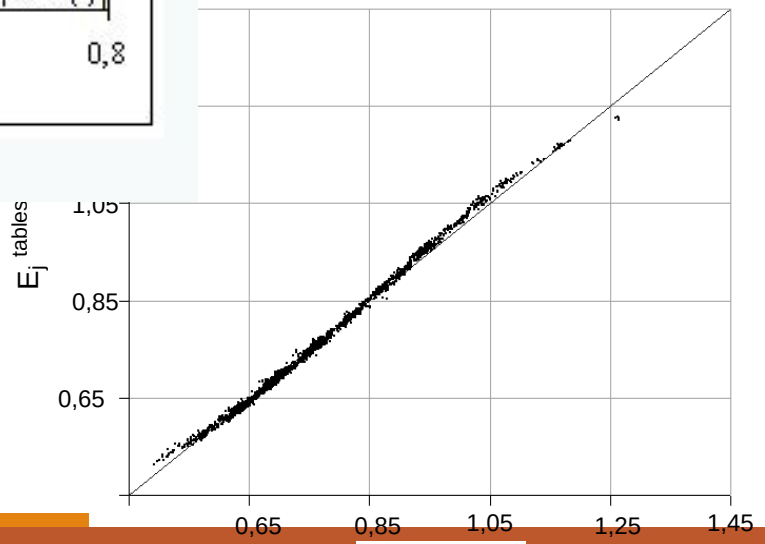
(20 + 1 integers)

2 1 2 2 0 2 1 1 2 1 1 2 0 0 1 1 1 2 2 0 0

Validation of AI system prediction in the 1nn approximation



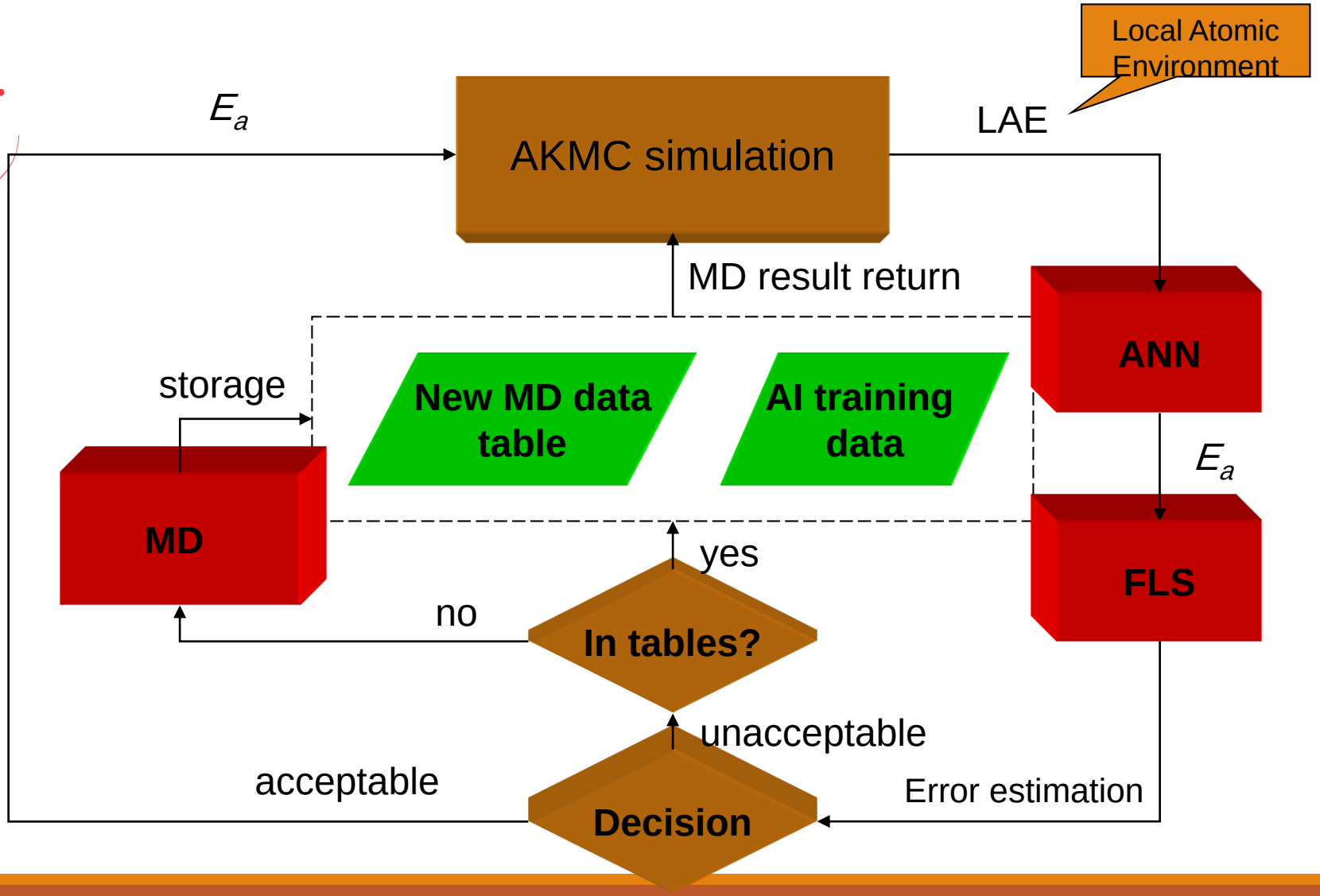
Energy barriers calculated by MD versus predicted by ANN for the same Local Atomic Environments



the maximum error committed by the ANN ≤ 8%,

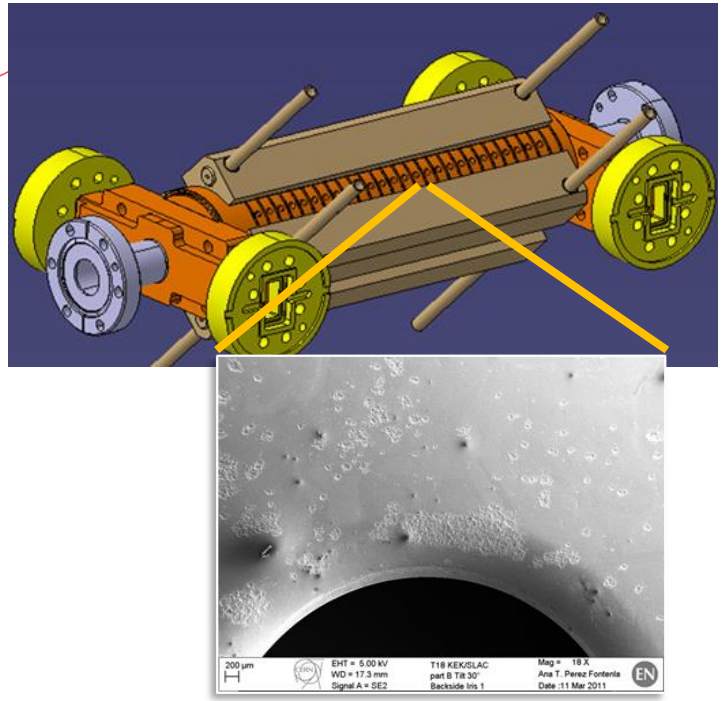
the average error = 5%,(≈ 0.05 eV)

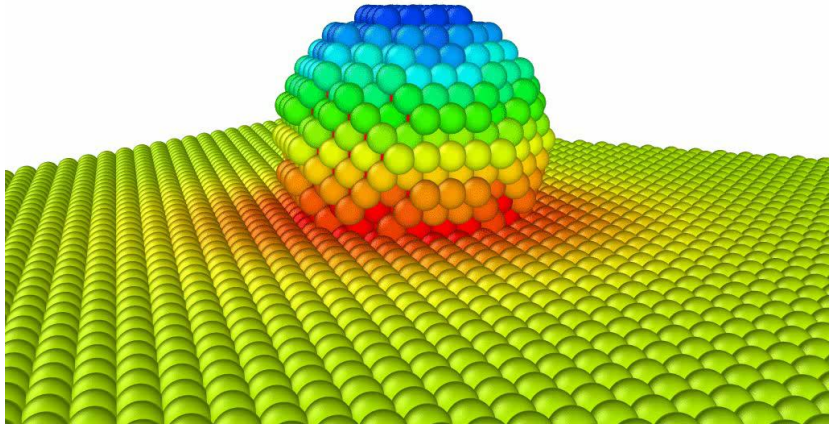
The structure of hybrid KMC code



Current interest: surface diffusion

We study self-roughening process on Cu surface in accelerating structures in CLIC:





To understand what happens on atomic level we have to model jumps of all atoms on Cu surface

Neural networks for Cu surface

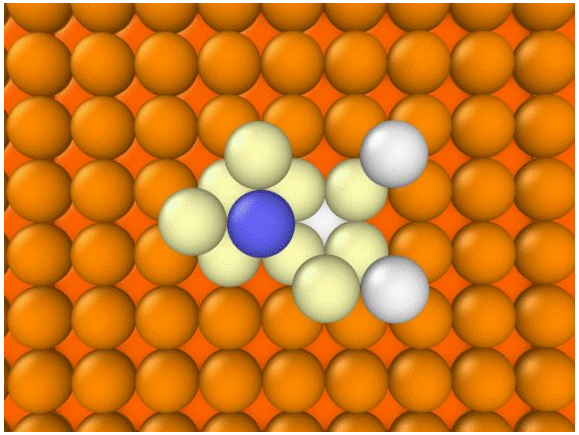
We calculate all barriers by nudged elastic band (NEB) method:

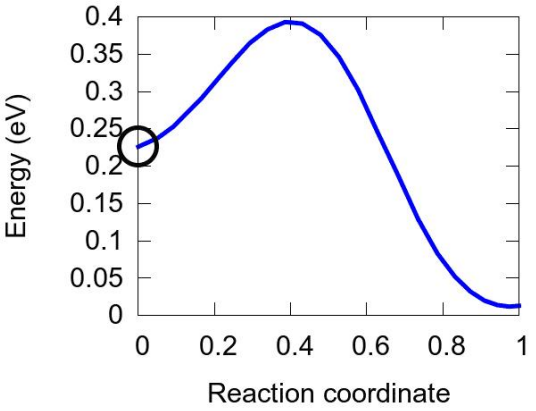
- Data from nudged elastic band (NEB) calculations:

```
...
1 0 1 1 1 0 0 0 1 1 1 0 0 1 0 1 0 0 1 0 1 1 0 0 0 0  0.331440022819
1 0 1 1 1 0 0 0 1 1 1 0 0 1 0 1 0 0 1 0 1 1 1 1 0 0  0.660164224842
1 0 1 1 1 0 0 0 1 1 1 0 0 1 0 1 0 0 1 1 1 0 0 0 0 0  0.480036427316
1 0 1 1 1 0 0 0 1 1 1 0 0 1 0 1 0 0 1 1 1 0 1 1 0 0  0.765357261622
1 0 1 1 1 0 0 0 1 1 1 0 0 1 0 1 0 1 1 0 1 0 0 0 0 0  0.272985753556
...
```

Input: 26-dimensional binary vector corresponding to a local atomic environment

Output: migration energy barrier





Jyri Lahitinen

NN for Cu surface diffusion

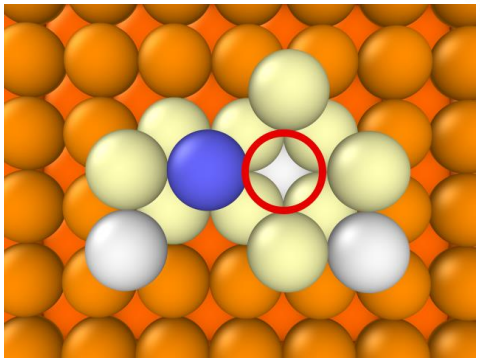
Model: multilayer perceptron with a single hidden layer

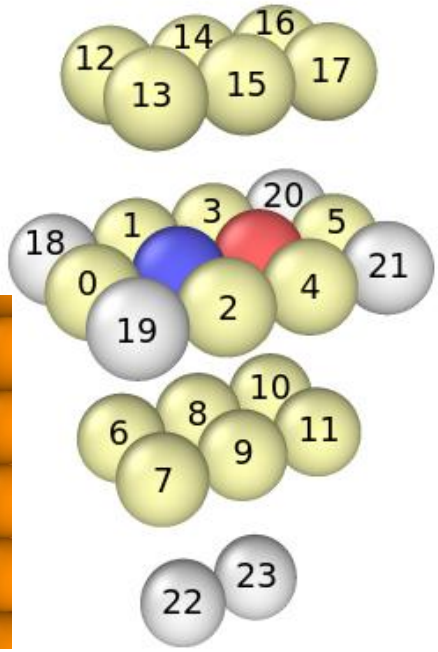
The initial set of 11.6 million data points is split into a training set and a validation set – early stopping

Additional tricks:

- Neural network ensembles
- Exclude symmetric cases
- Separate networks for different parts + classifier

LAE

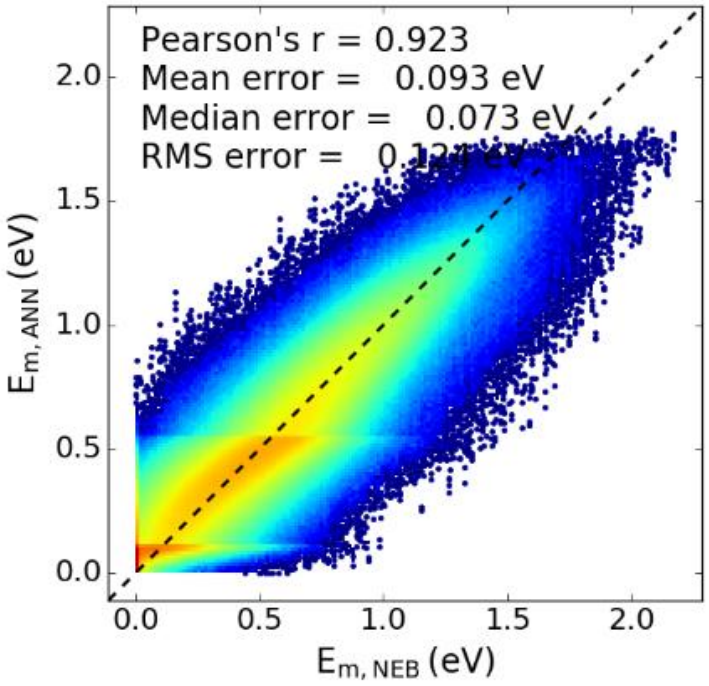




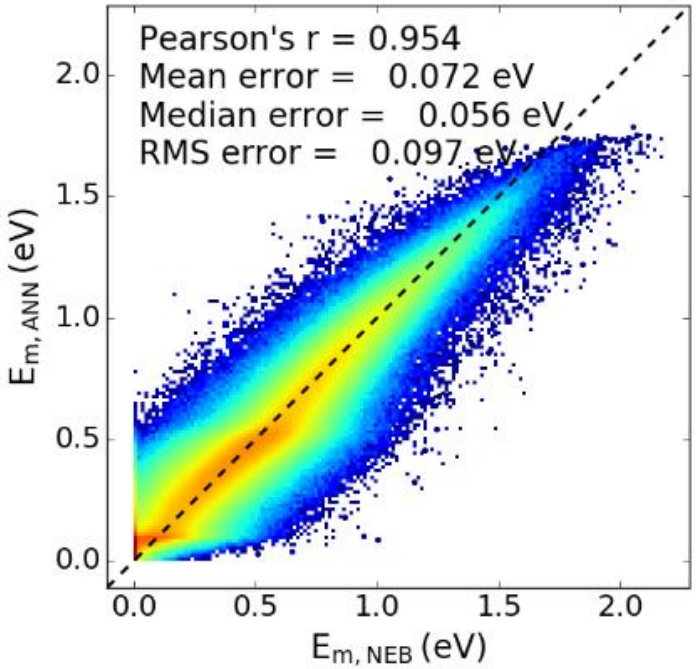
Results of neural nework predictions

Using different tricks to help NN to recognize he pattern, we have achieved a somewhat improvement:

Full data set, no tricks

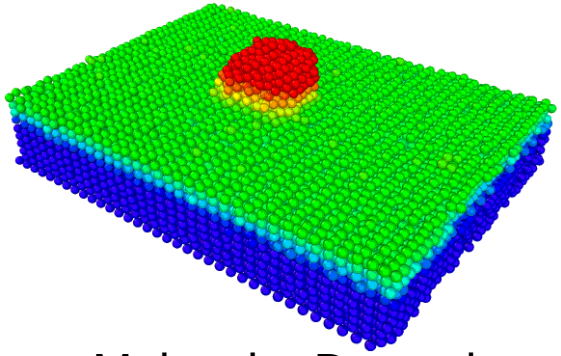


Using ensembles, symmetry, classifier

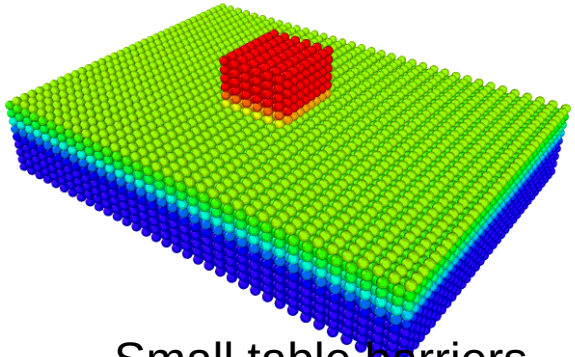


If the barriers are wrong

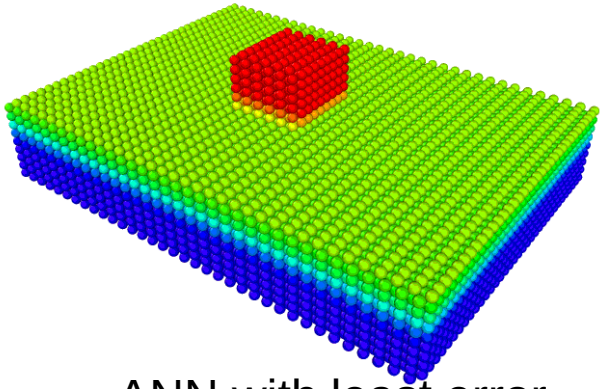
What will happen if the ANN predicts barriers inaccuratel



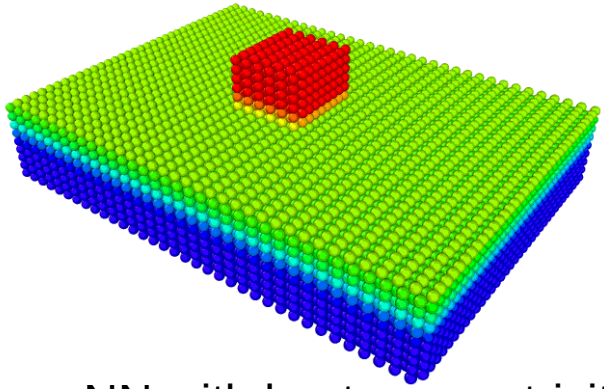
Molecular Dynamics



Small table barriers



ANN with least error



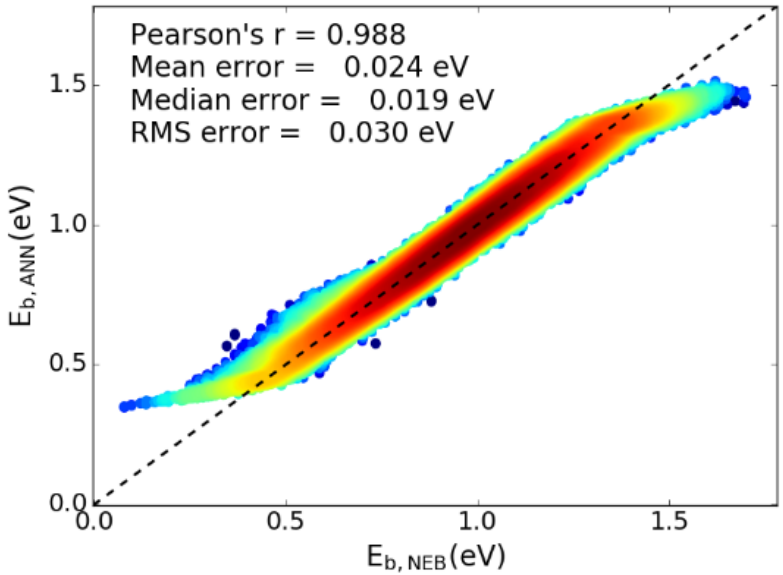
NN with best symmetricity

Back to bulk: ANN performance improves

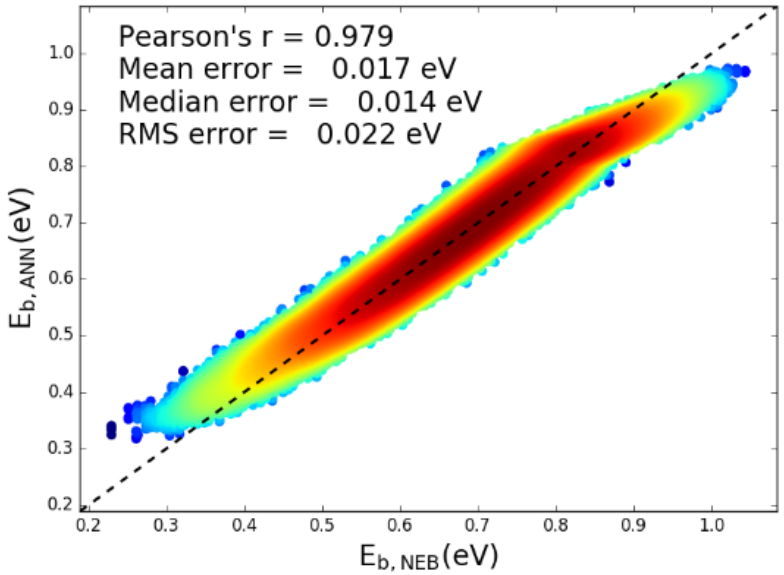
Ni-rich NiCr nanoparticles exhibit sharply dropping Curie temperature with increasing Cr concentration

This phenomenon can be used for cancer treatment by tuning Curie temperature to as low as 40-60 °C for e.g. magnetic hyperthermia?

Ni jumping

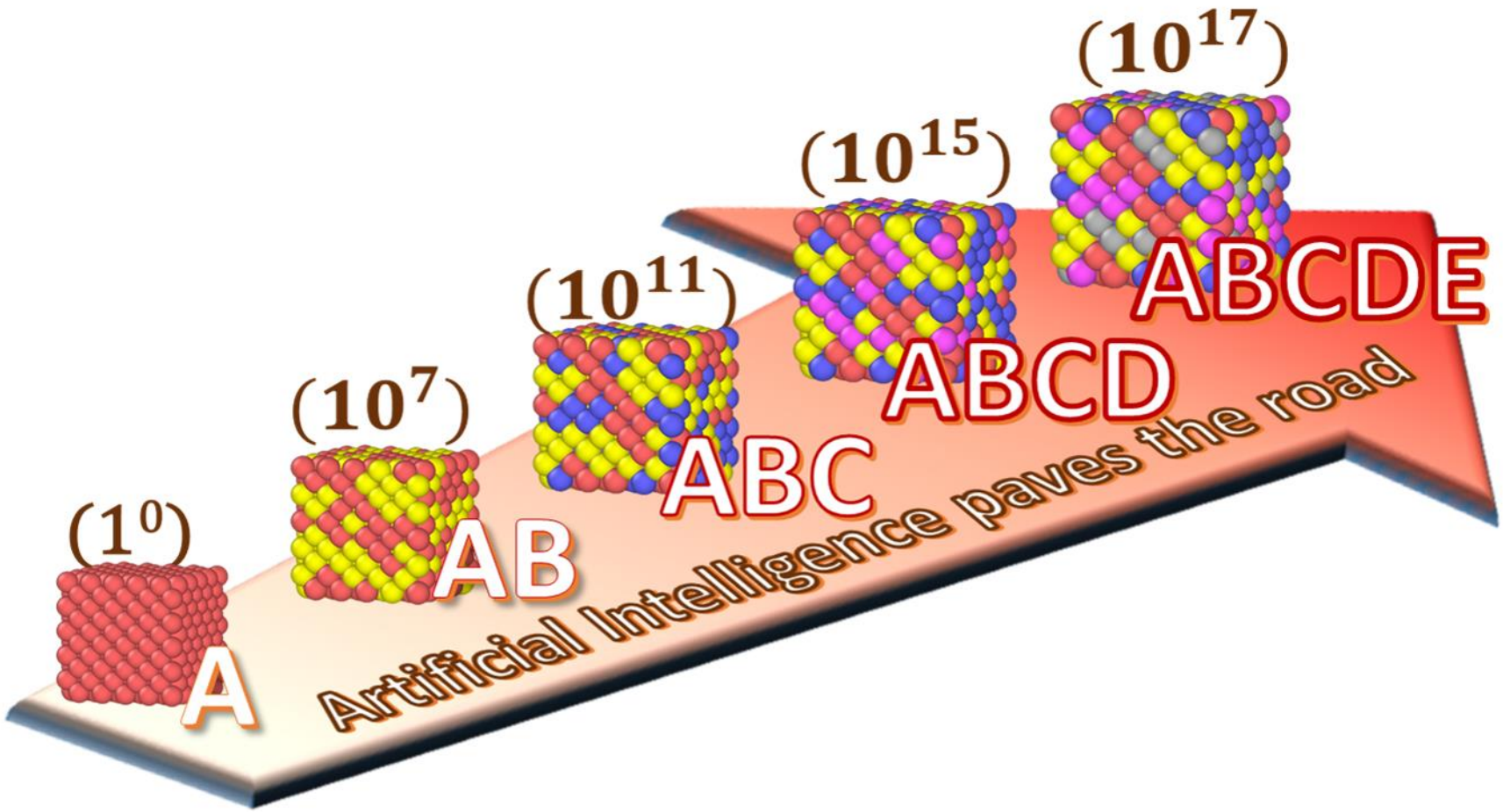


Cr jumping



Adding complexity

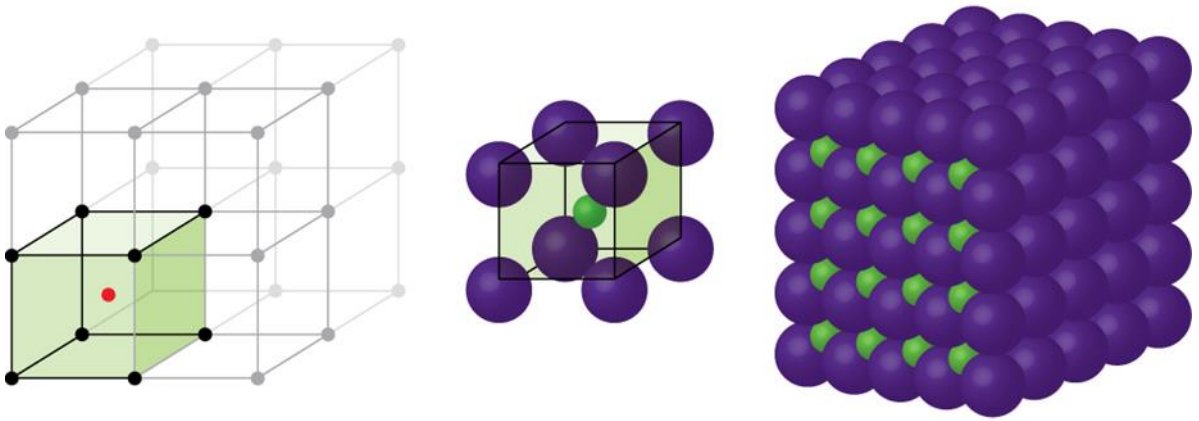
High Entropy alloys are materials with more than 5 elements:



Summary

In Materials Research, we are collecting more and more data with or without help of computers

It is time to teach the computers the logic hidden in the data that we can learn more and faster about exciting new materials and start implementing them in the real life!



Body-centered simple cubic structure