Development of physically informed neural network (PINN) interatomic potentials

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Motivation

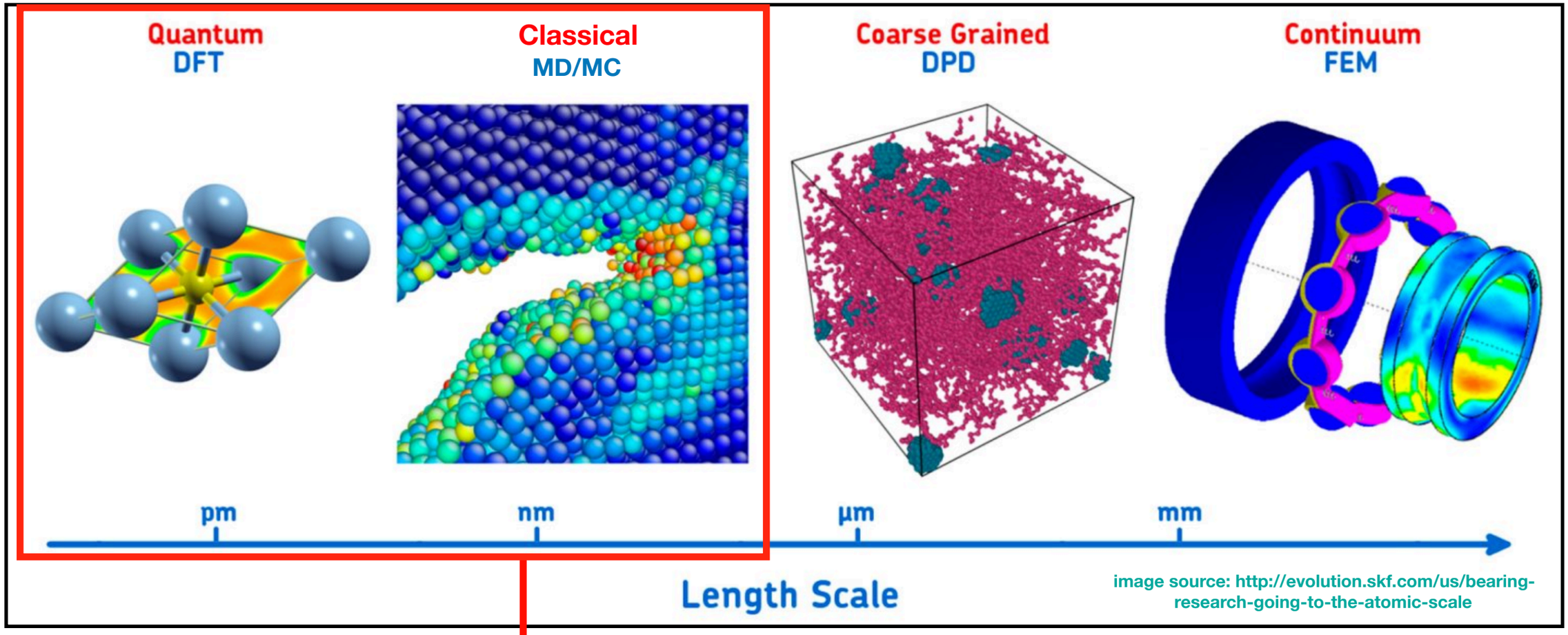


image source: http://evolution.skf.com/us/bearing-research-going-to-the-atomic-scale

Ab-initio/DFT

- Slow
- Size limited (N~10^2)
- 0K or short timescales
- Very accurate

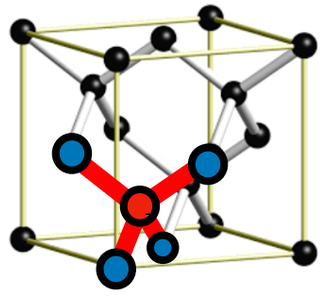
Compromises

Speed
Accuracy
Scalability
Transferability

Better potential models

Classical (MD/MC)

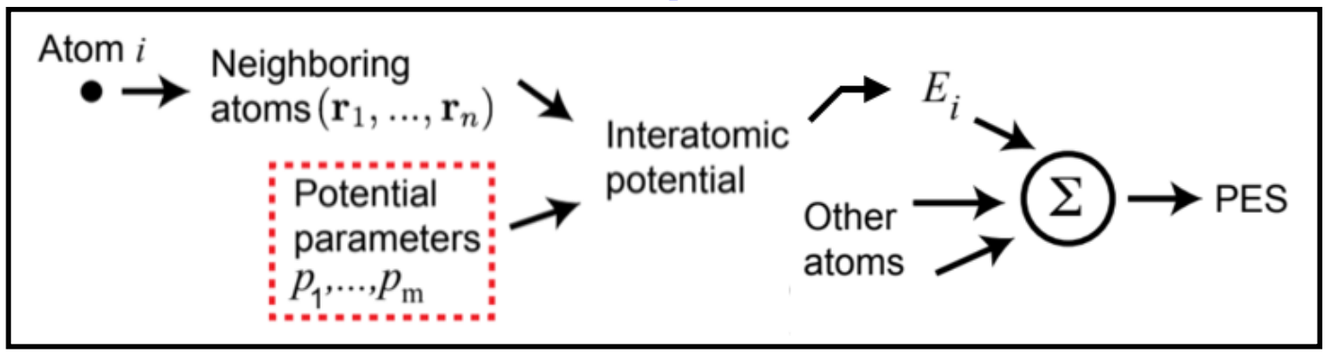
- Computationally Fast
- Larger systems (N~10^7)
- Kinetic phenomena/long simulations
- ★Accuracy depends on *approximation* of the potential energy surface (PES)



$$E = E(\mathbf{r}_1, \ldots, \mathbf{r}_N)$$

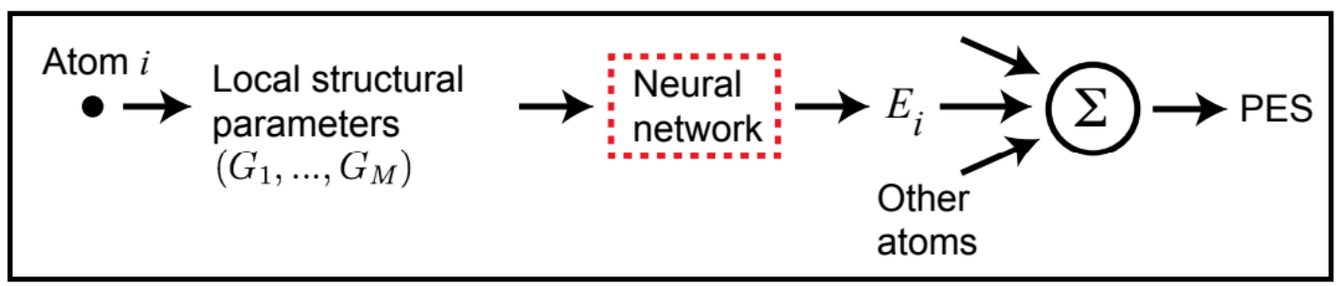
Interatomic potential model types

Traditional interatomic potential:



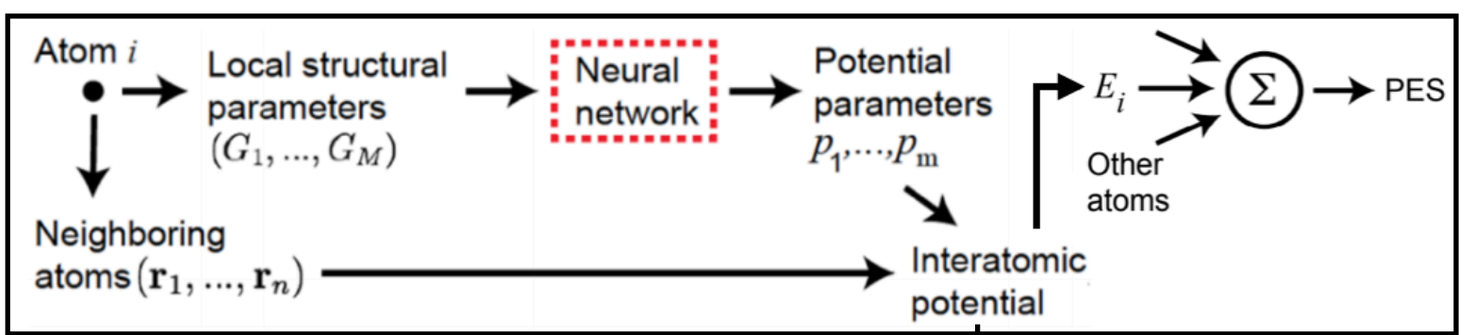
- **LJ, EAM, ADP, Tersoff, REAX … etc**

"Mathematical" or "straight" NN potentials:



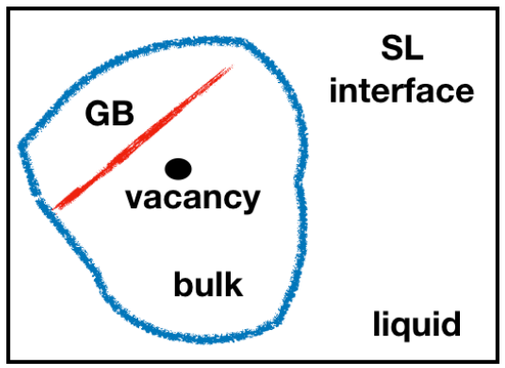
- **Machine learning potentials**
  - **Gaussian process regression**
  - **Interpolating moving least squares**
  - **Kernel ridge regression**
  - **Compressed sensing**
  - **ANN potentials**

Physically informed neural network (PINN):



local parameterization

Pros	Cons
• Fast • Decent extrapolation • Physically inspired	• Difficult to train/fit • Hard to improve upon once finalized • Accuracy limitations
• Fast relative to DFT • DFT level accuracy (~1-5 mEv) within training set • Relatively straight forward/routine to train/fit • Systematic improvement (add more data)	• Slower than traditional potentials • Bad extrapolation
• Same as straight NN • Decent extrapolation • Physically inspired	• Slower than traditional potentials



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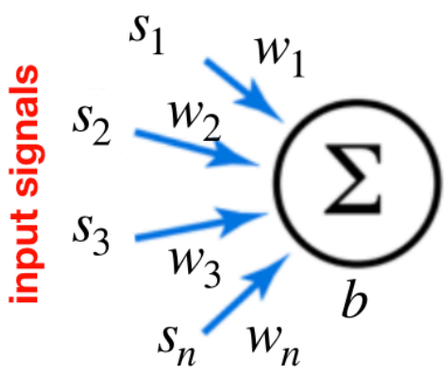
Physically informed artificial neural networks for atomistic modeling of materials
GPP Pun, R Batra, R Ramprasad, Y Mishin - Nature communications, 2019

Artificial neural networks

Artificial neuron

AKA: nodes or perceptrons



weighted and biased signal

$$s = \Sigma_i w_i s_i + b$$

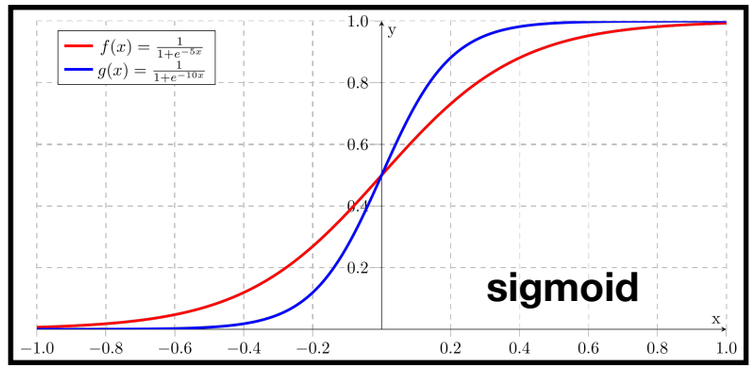
Activation function

$$f(s) = \frac{1}{1 + e^{-s}}$$

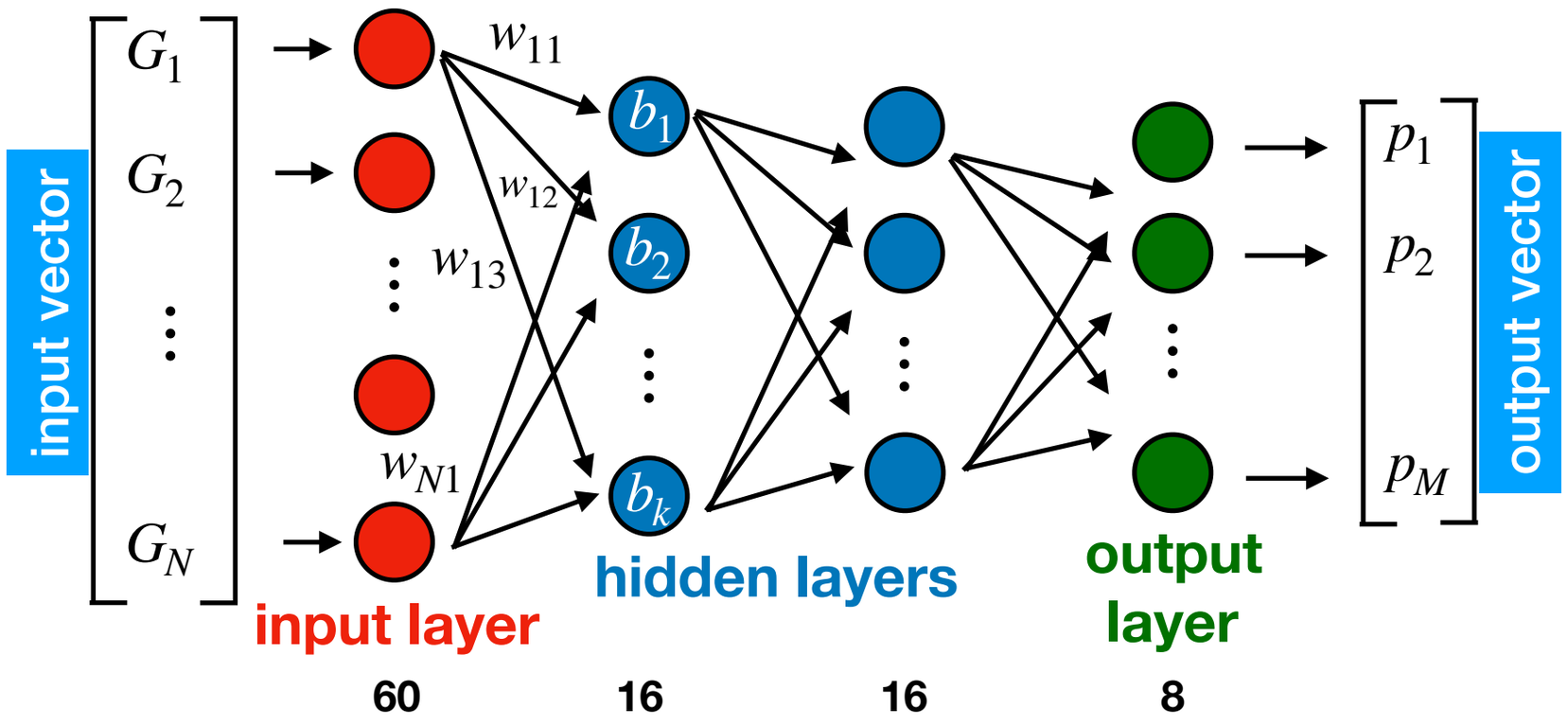
$$f(s)$$

neuron output

Activation function



Artificial neural network



Training

known inputs $\mathbb{R}^N$ → NN → known outputs $\mathbb{R}^M$

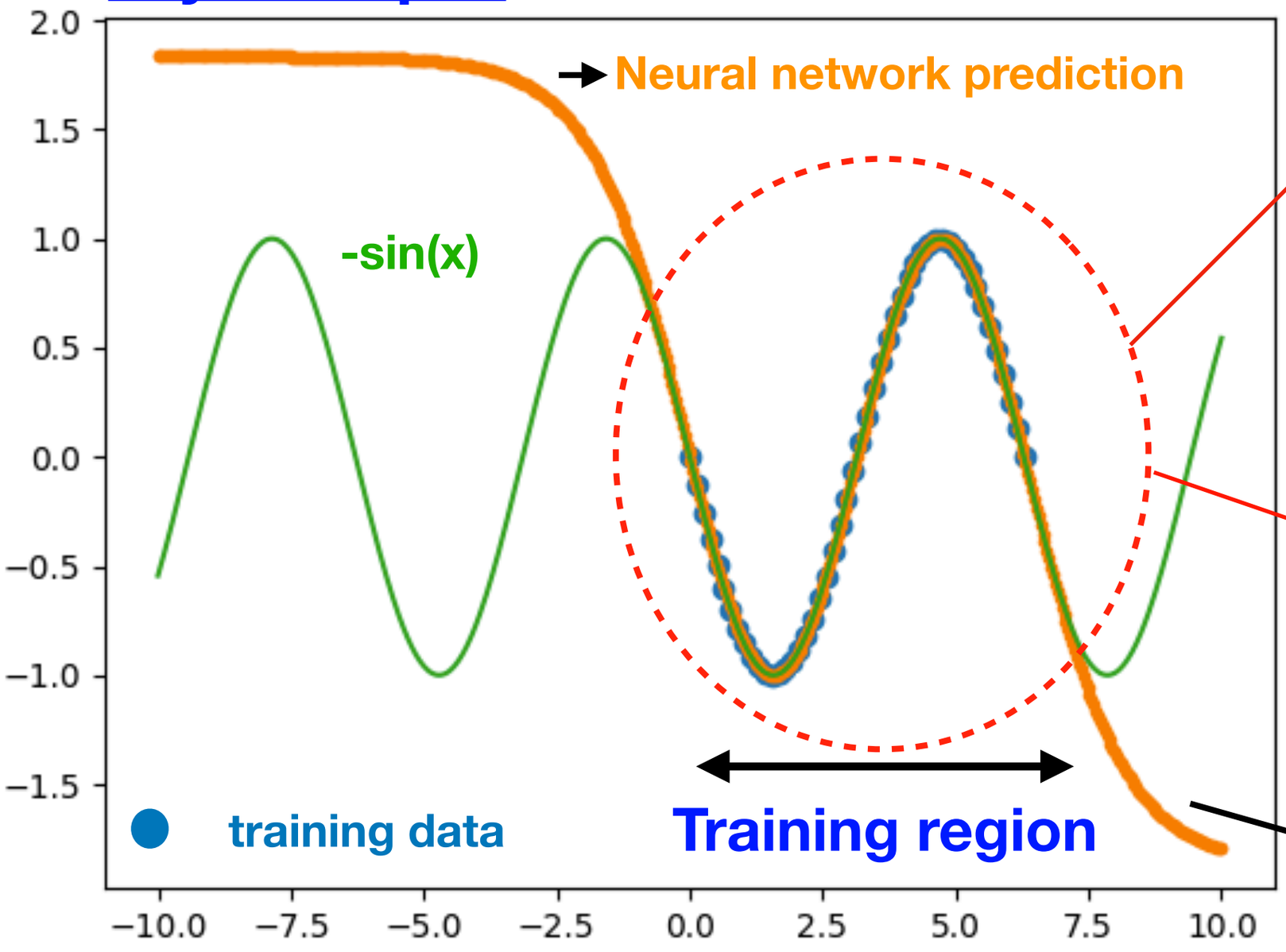
fit/optimize weights and biases

data:

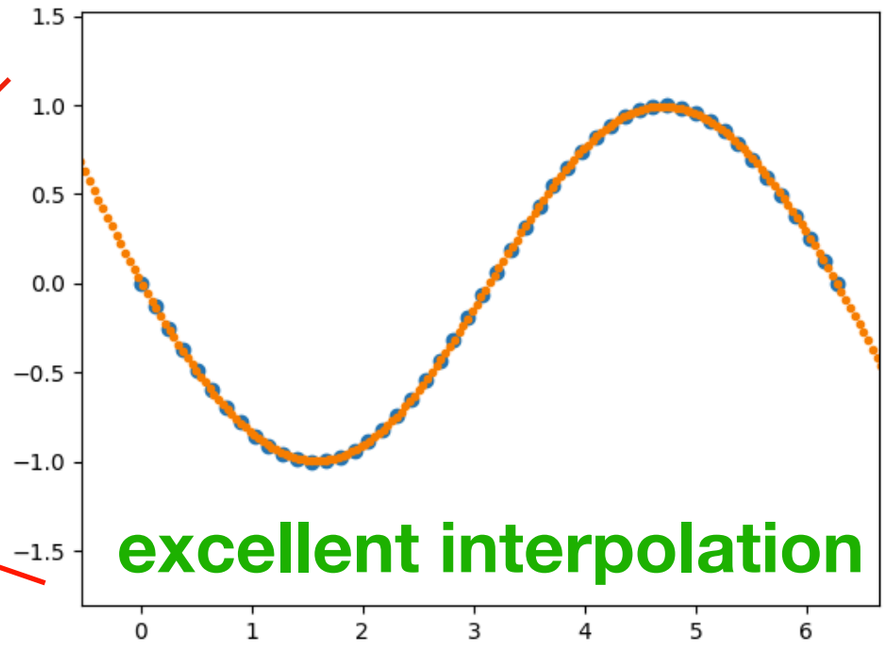
The weights and bias are the NN's fitting parameters (~1500 parameters)

Artificial neural networks

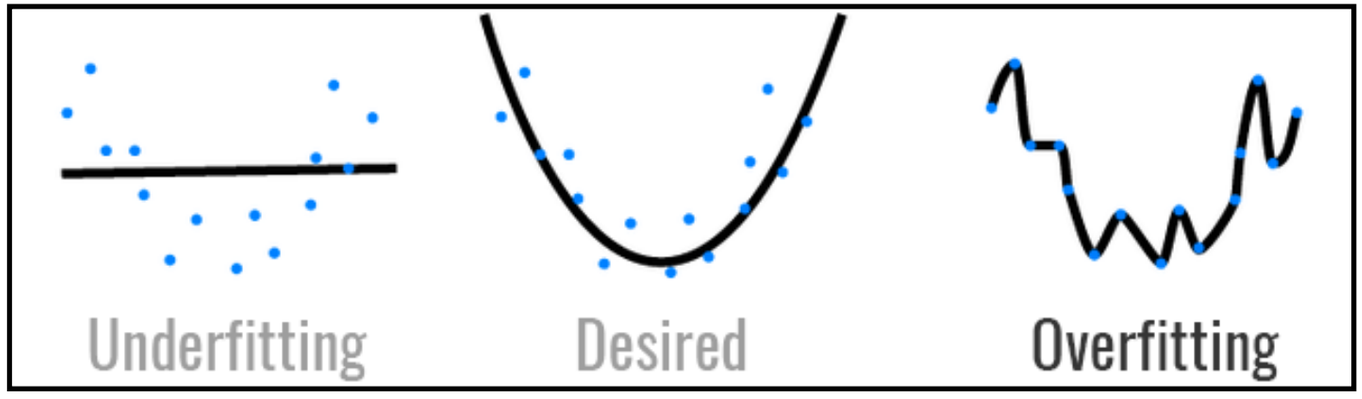
Toy example:



Train NN to reproduce provided data



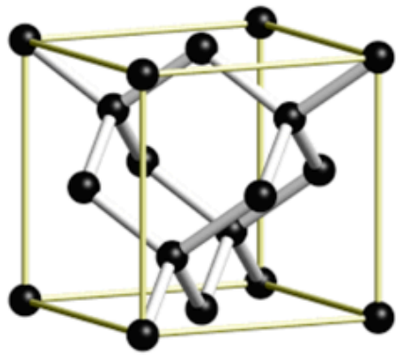
unable to extrapolate

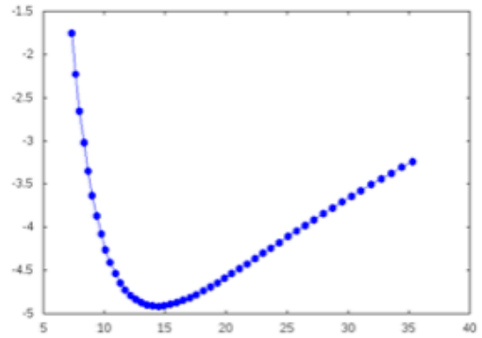


Physically informed neural network potential (PINN)

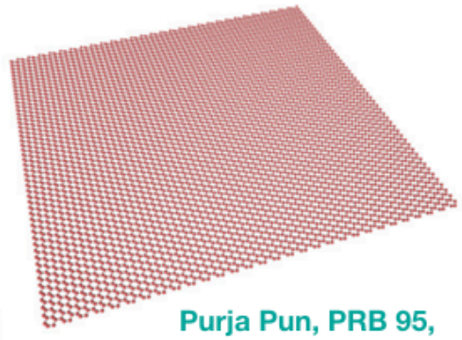
Training/test set generation

Stable structure: (Diamond)

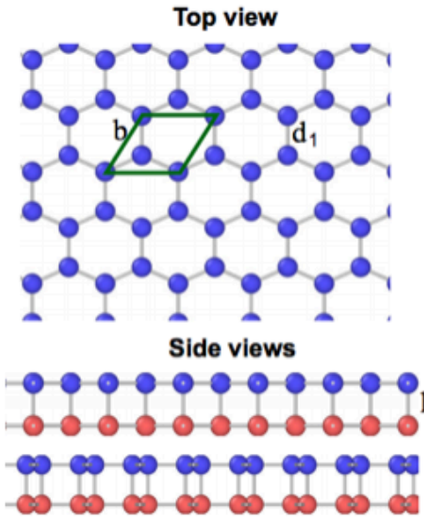




Two dimensional structures:

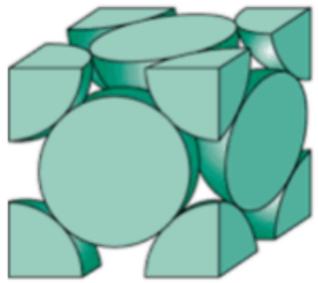


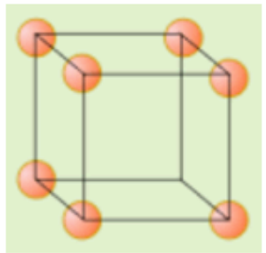
Purja Pun, PRB 95, 224103 (2017)

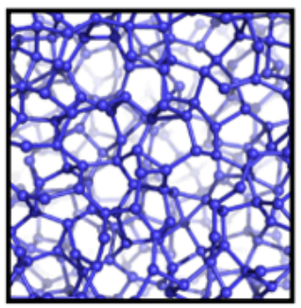


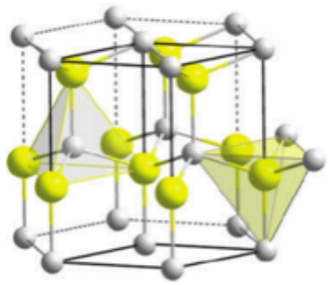
6 silicene allotropes

Alternative structures:









~14 alternate structures

- FCC, BCC, HEX, HCP, SC, Liquid, Amorphous …etc

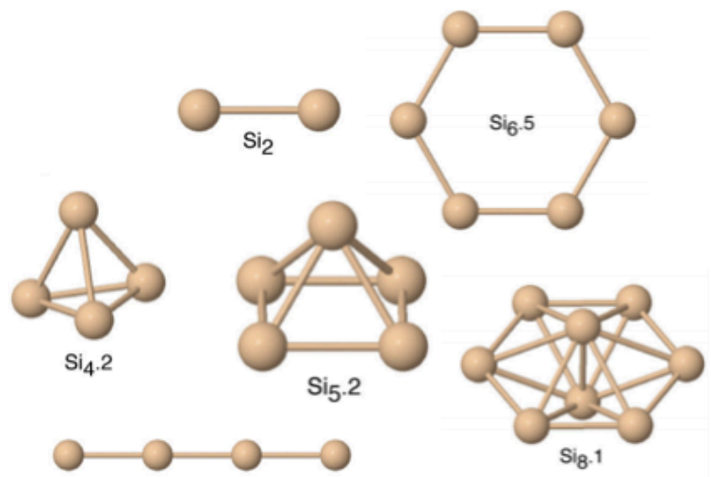
DFT calculation details

- Functional/PP: PBE/PAW
- ENCUT=600 eV
- ~4300 structures
- block size 1-96 atoms
- k-point convergence tests for each group

Non-equilibrium sampling

- Isotropic expansions/compressions
- Random local atomic perturbations
- Anisotropic box variations

Clusters:

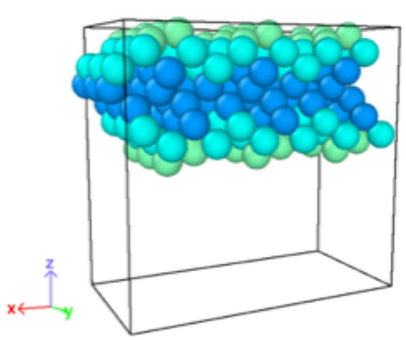


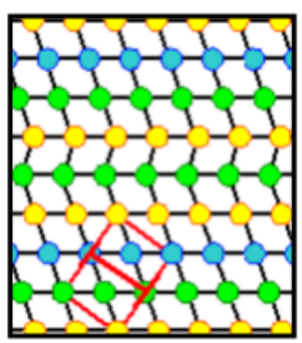
Purja Pun, PRB 95, 224103 (2017)

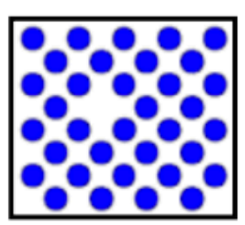
~18 atomic clusters

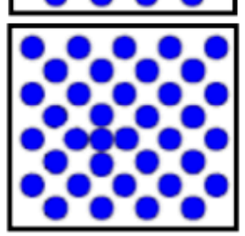
- DFT data is shifted so DC phase coincides with -4.63

Defects:









~27 different defects

- Vacancies, Various self interstitials, Surfaces, Stacking faults

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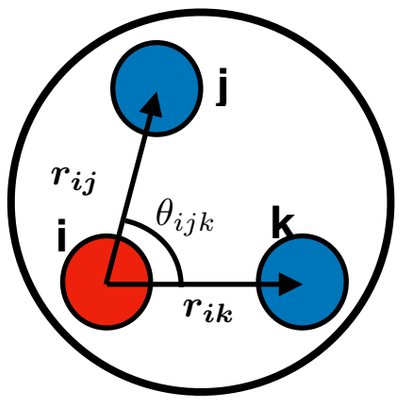
Traditional BOP potential



$$E_i = \frac{1}{2}\left(\Sigma_{j\neq i} e^{A_o - \alpha_o r_{ij}} - S_{ij} b_{ij} e^{B_o - \beta_o r_{ij}}\right) f_c(r_{ij}) + E_p$$

cutoff function

promotional energy

Model can be used for Metallic or covalent systems

bond order parameter $b_{ij} = (1 + z_{ij})^{-\frac{1}{2}}$

$$E_p = -\sigma_o \left(\Sigma_{j\neq i} S_{ij} b_{ij} f_c(r_{ij})\right)^{\frac{1}{2}}$$

$$z_{ij} = a_o \Sigma_{k\neq i,j} S_{ik} (cos(\theta_{ijk} + h_o)^2 f_c(r_{ik})$$

$$S_{ijk} = 1 - f_c(r_{ik} + r_{jk} - r_{ij}) e^{-\lambda_o (r_{ik} + r_{jk} - r_{ij})}$$ screening $$S_{ij} = \prod_{k\neq i,j} S_{ijk}$$

step-0:

Fit a baseline traditional potential via 8 adjustable $(A_o, B_o, \alpha_o, \beta_o, a_o, h_o, \lambda_o, \sigma_o)$

Training process:

pytorch

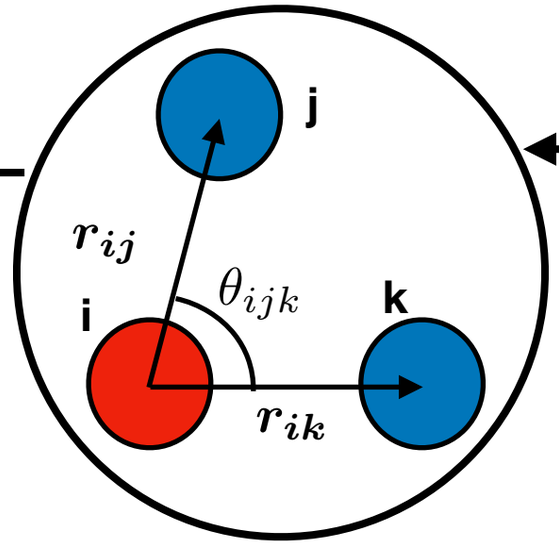
	"Training set"		Model error
	Structures	DFT energies	Model energies
	structure-1	E_1	$\tilde{E}_1$
	structure-2	E_2	$\tilde{E}_2$
	⋮	⋮	⋮
	structure-N	E_N	$\tilde{E}_N$

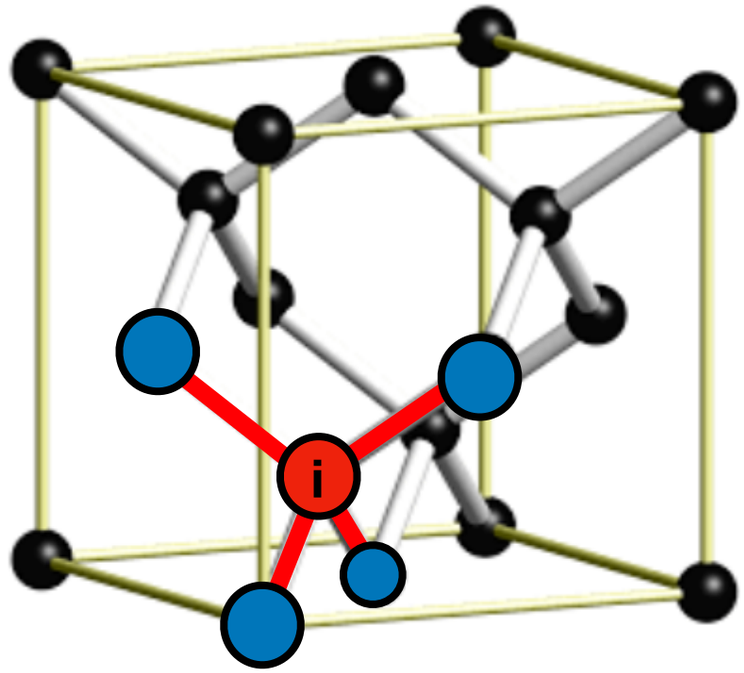
$$RMSE = \left(\frac{\Sigma_s (E_s - \tilde{E}_s)^2}{N}\right)^{\frac{1}{2}}$$

Local structure parameters

Structure parameters:

$$G_i^{m,n} = \sum_{j,k} P_m(cos(\theta_{ijk}))f(r_{ij})f(r_{ik})$$





Angular term:

$P_m(cos(\theta))$ $m = 0,1,2,4,6$

(Legendre polynomials)

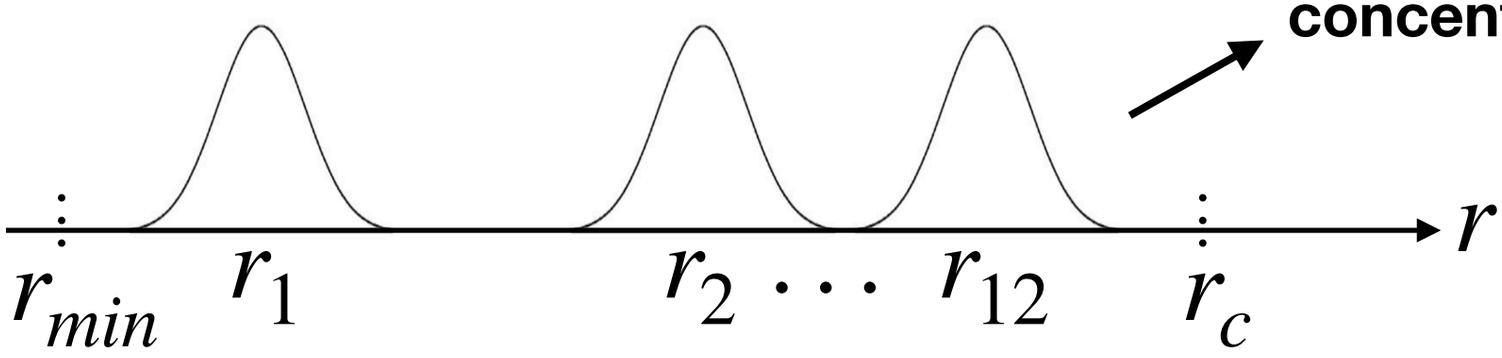
Radial term:

$$f(r) = \frac{1}{r_n} e^{-\frac{(r-r_n)^2}{\sigma^2}} f_c(r)$$

choose 12 values for r_n

$f_c(r)$ = Cutoff function

$$f_c(r) = \begin{cases} \dfrac{(r-r_c)^4}{d^4 + (r-r_c)^4} & r \le r_c \\ 0, & r \ge r_c \end{cases}$$



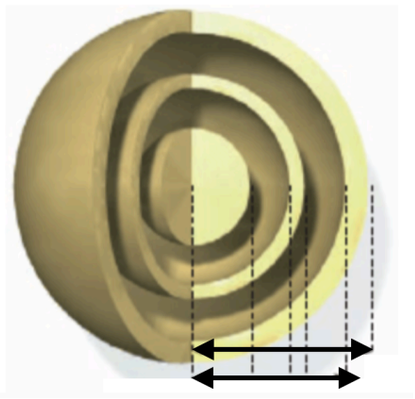
Gi's act as "fingerprints" of the local atomic environment

$8\, r_n$ *with* $5 P_m$

$\downarrow$

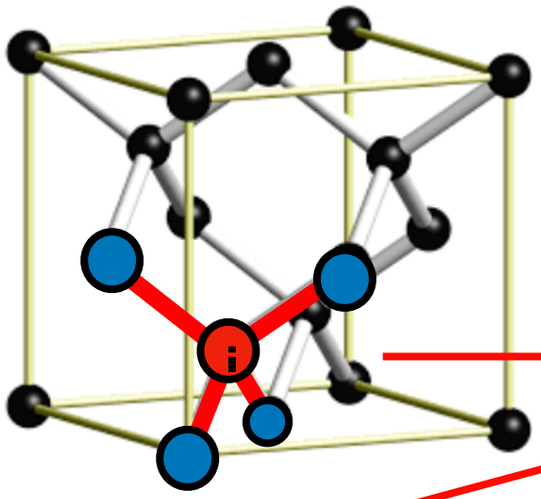
$G_i^{m,n} = [40 \times 1]$ for each atom

concentric shells



PINN potential model

Energy of atom-i



neighboring atom positions

$(r_1, r_2 \ldots r_n)$

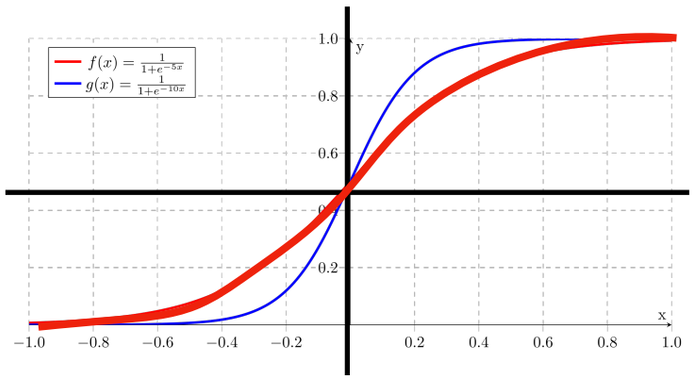
$G_1 = G_1(r_{ij}, \theta_{ikj})$

$G_2 = G_2(r_{ij}, \theta_{ikj})$

Local structure parameter calculation

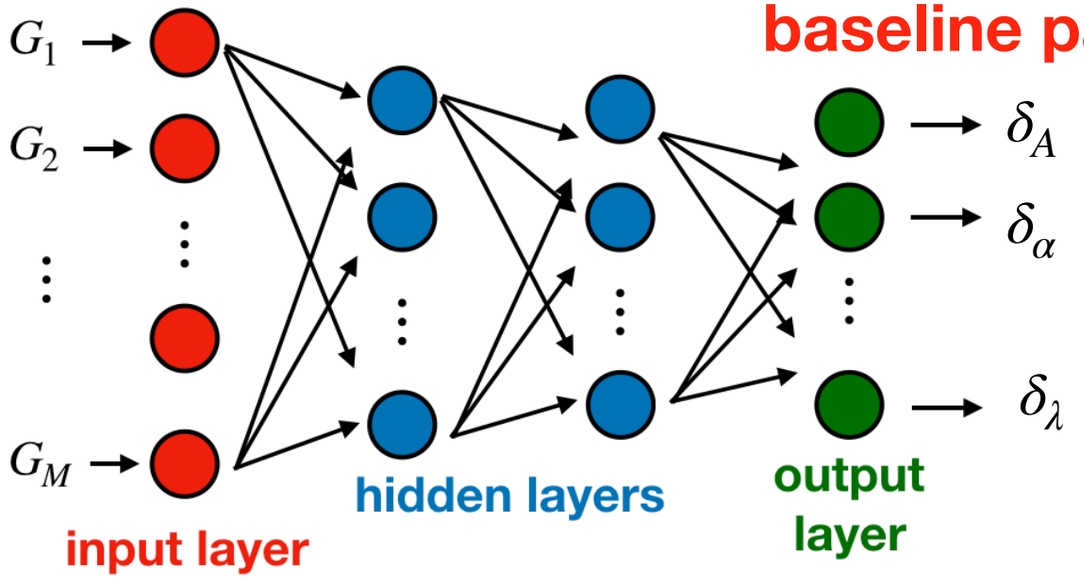
structural "fingerprints"

$(G_1, G_2 \ldots G_M)$



$$A(x) = \frac{1}{e^{-x}+1} - \frac{1}{2}$$

perturbations to baseline parameters



$$(A_o, B_o, \alpha_o, \beta_o, a_o, h_o, \lambda_o, \sigma_o)$$ baseline parameters

$+$

$$(\delta_A, \delta_B, \delta_\alpha, \delta_\beta, \delta_a, \delta_h, \delta_\lambda, \delta_\sigma)$$ NN perturbation

$=$

$$(A_i, B_i, \alpha_i, \beta_i, a_i, h_i, \lambda_i, \sigma_i)$$ atom-i parameterization

Training:

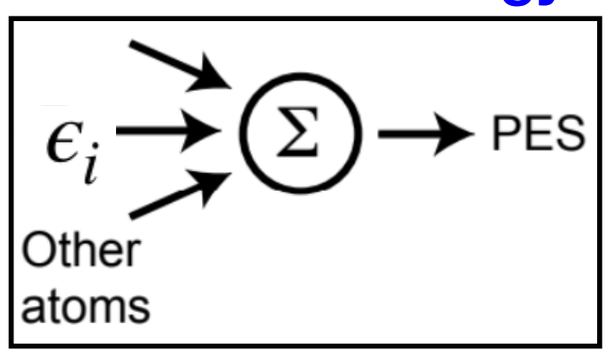
$$RMSE = \left(\frac{\Sigma_s (E_s - \tilde{E}_s)^2}{N} \right)^{\frac{1}{2}} = NN(w, b)$$

Find the NN weights and bias's which minimize the RMSE

BOP Model

atomic energy → ϵ_i

Structure's energy



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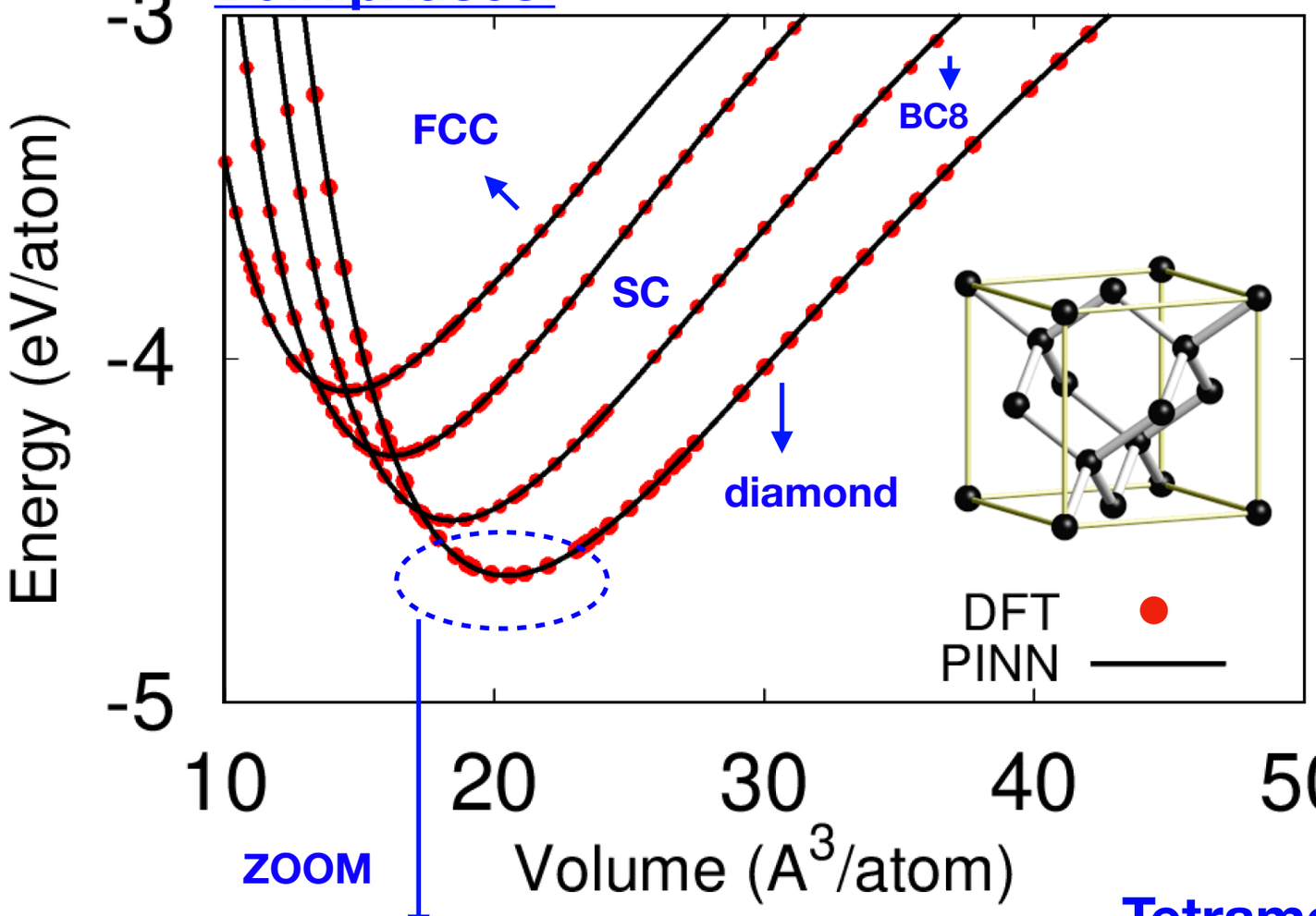
Results

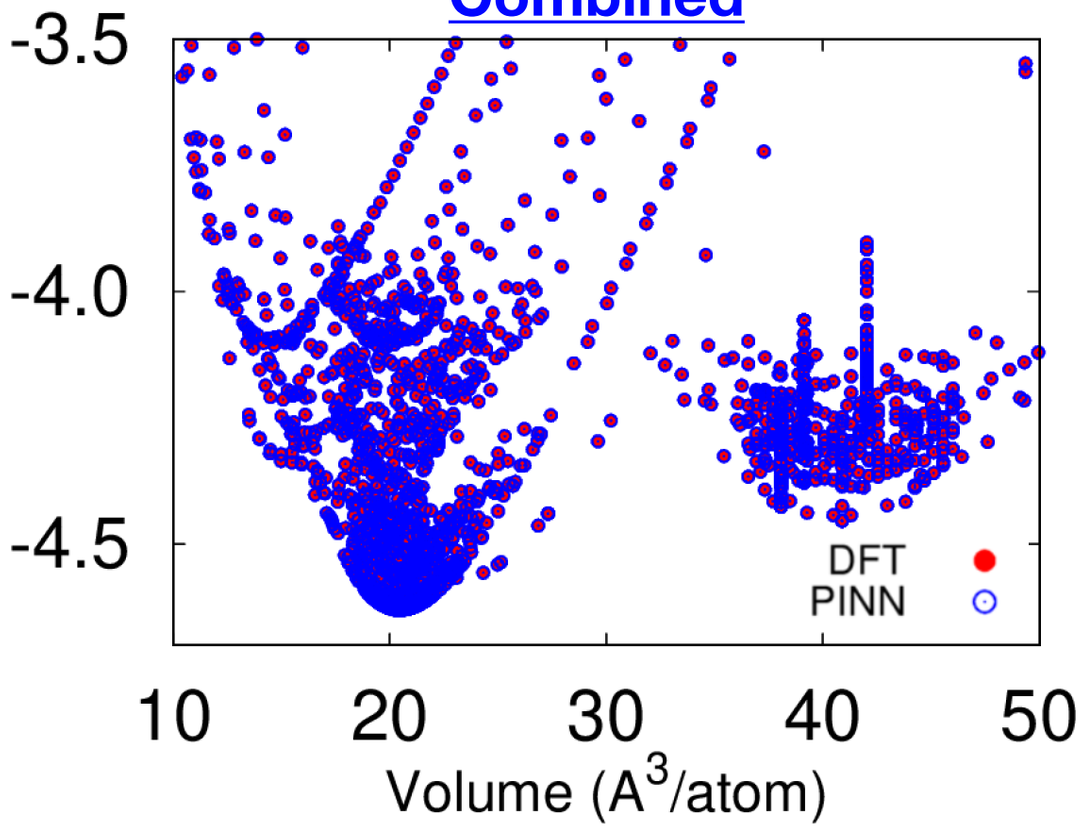
Volume-energy curves

NN: 60x32x8

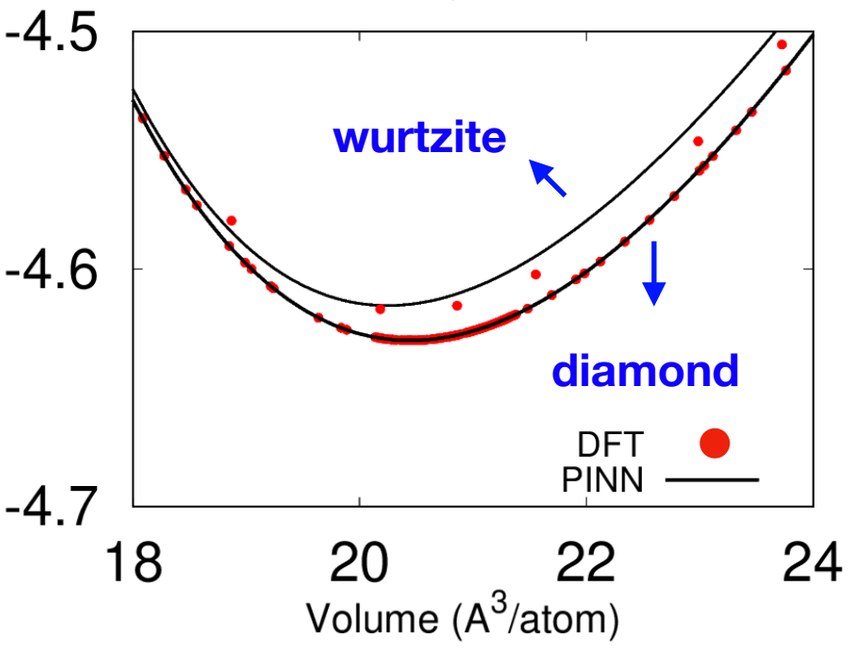
Bulk phases:



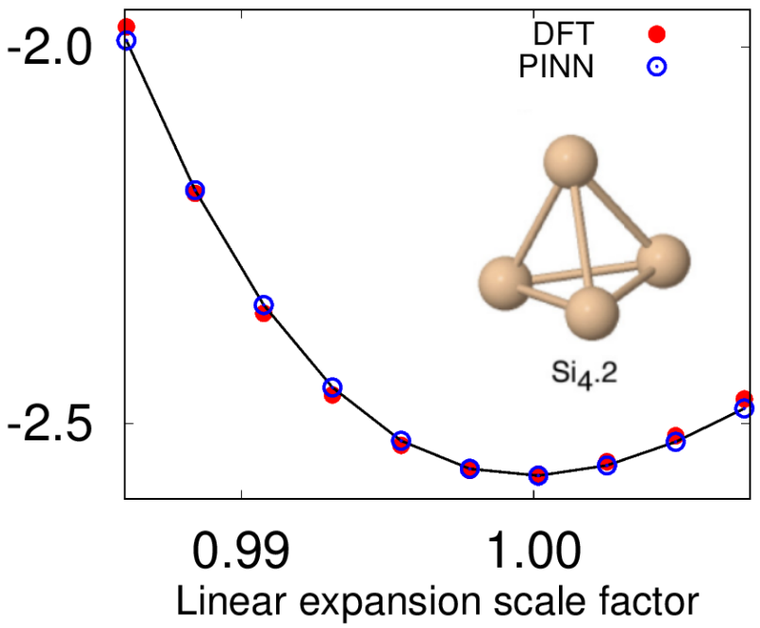
Combined



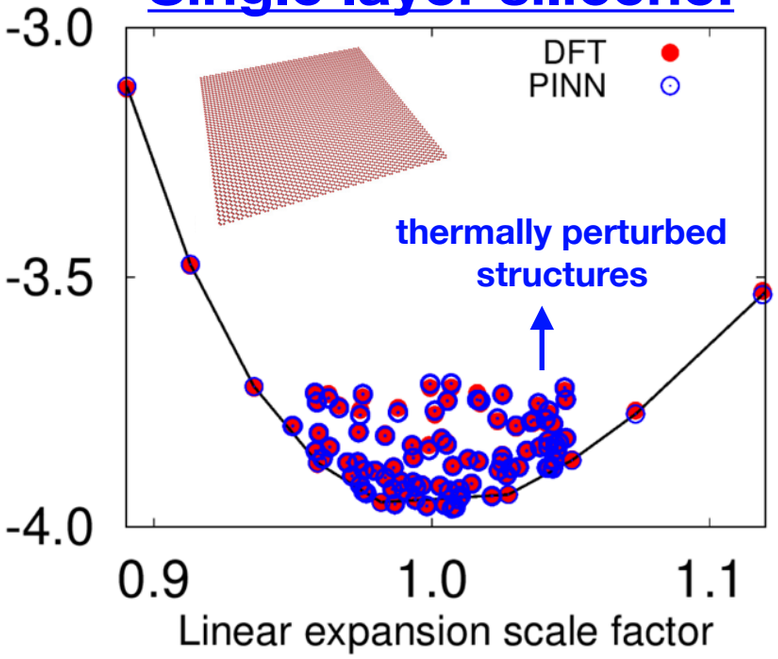
ZOOM



Tetrameter



Single layer silicene:



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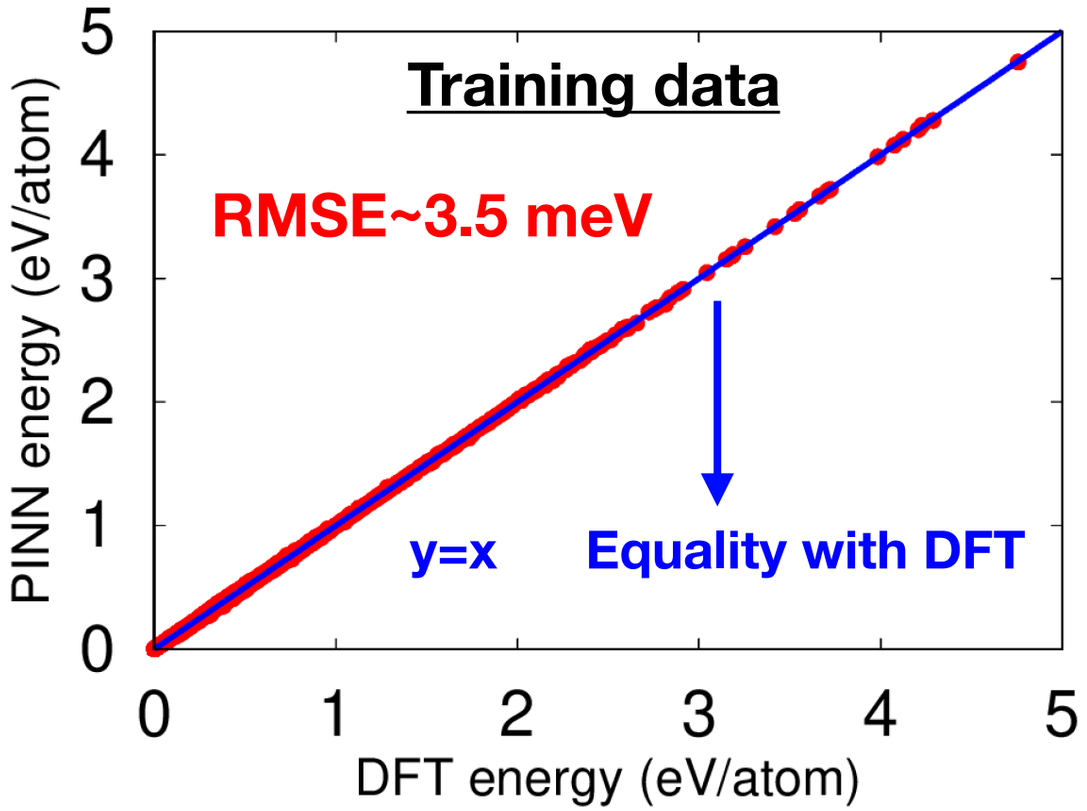
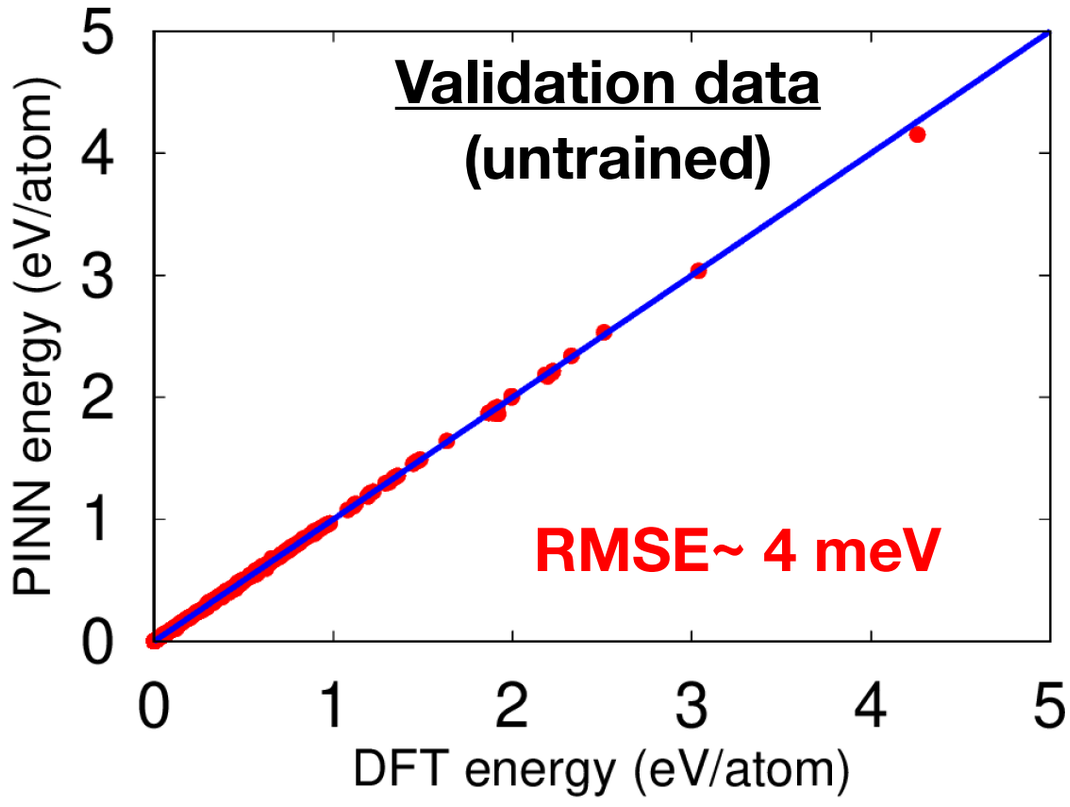
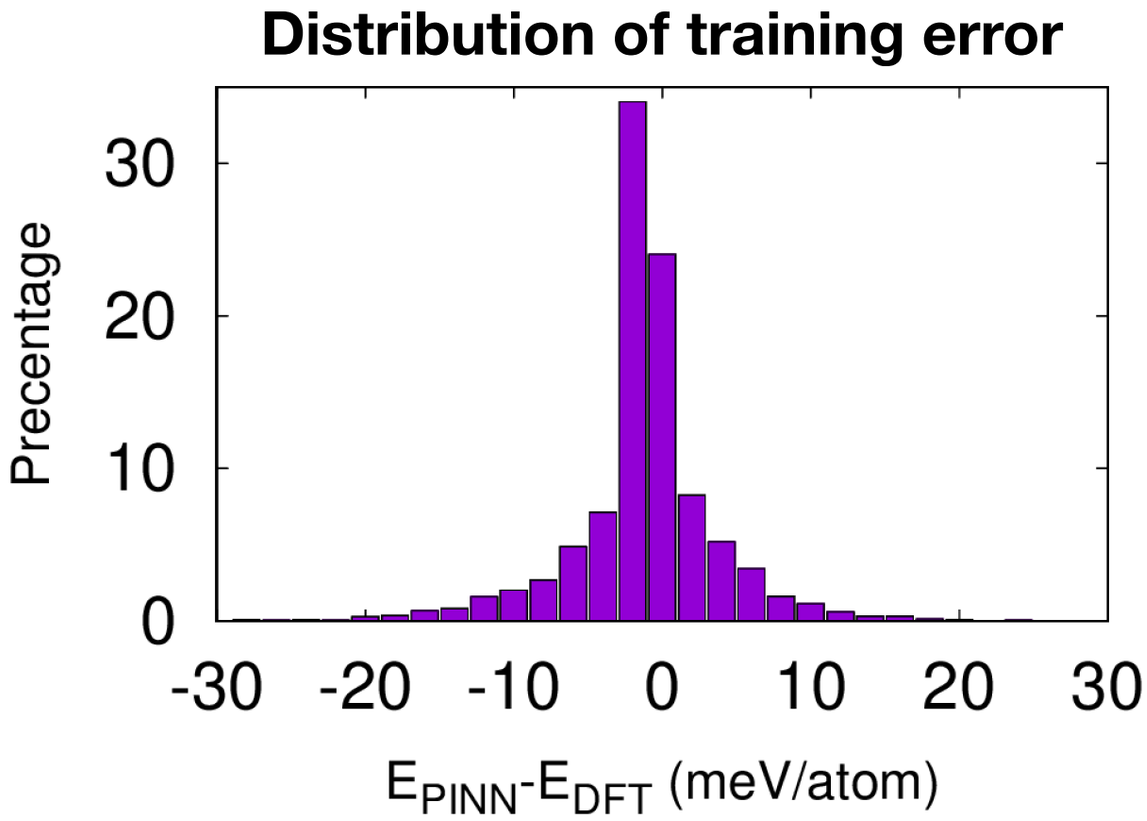
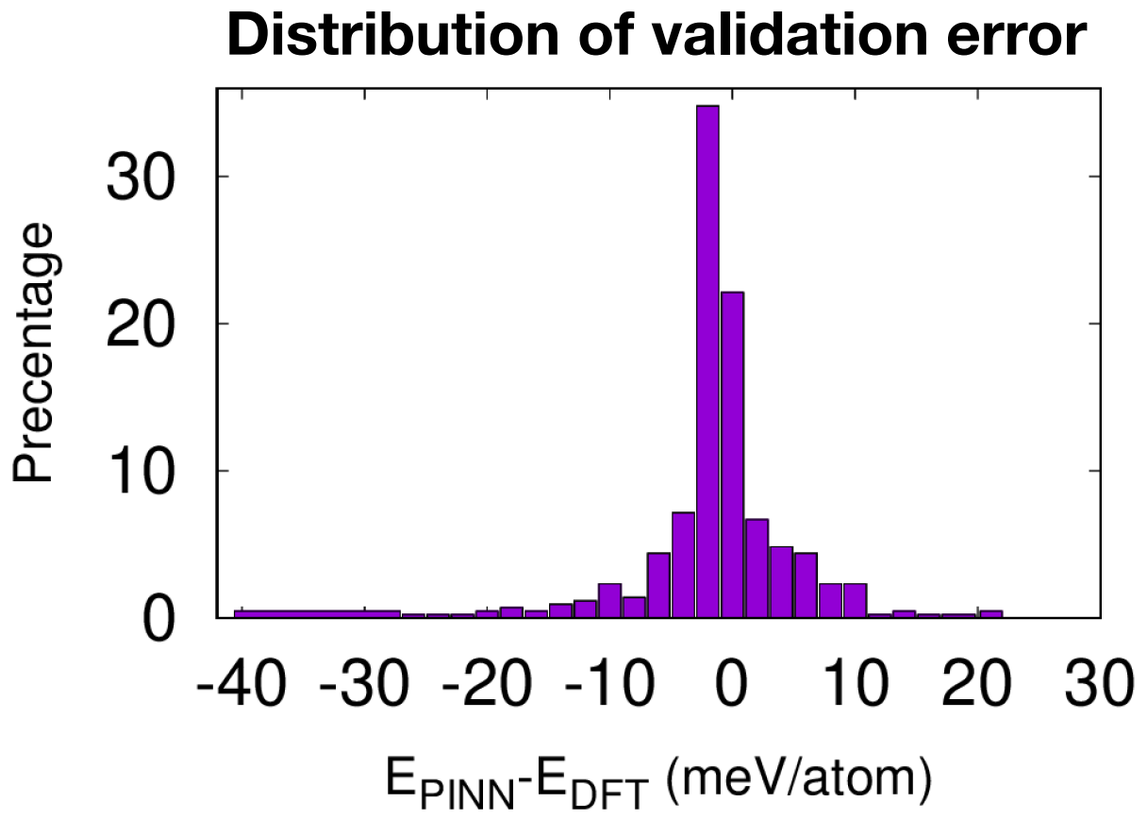
Reproduction of DFT energy landscape









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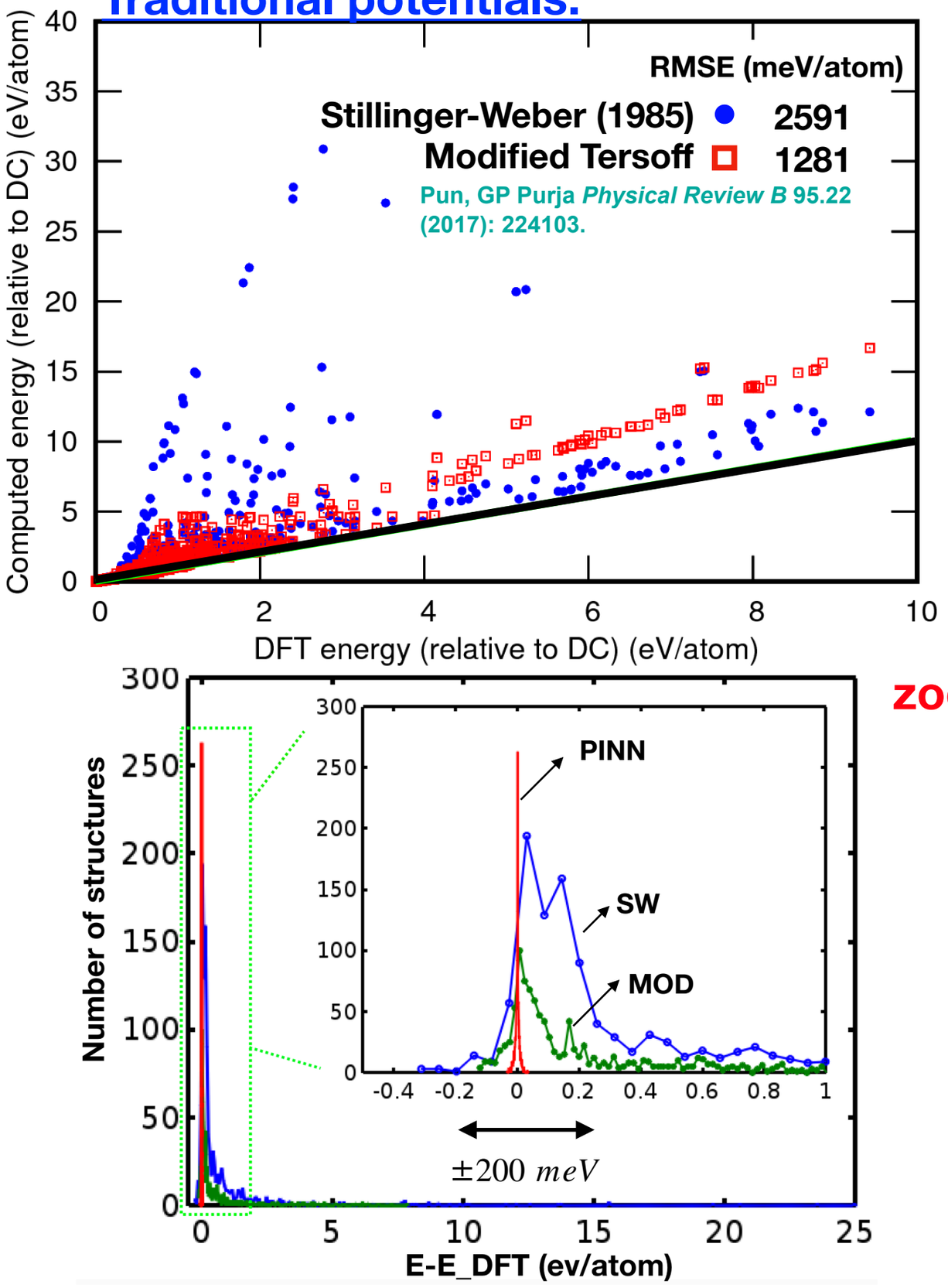
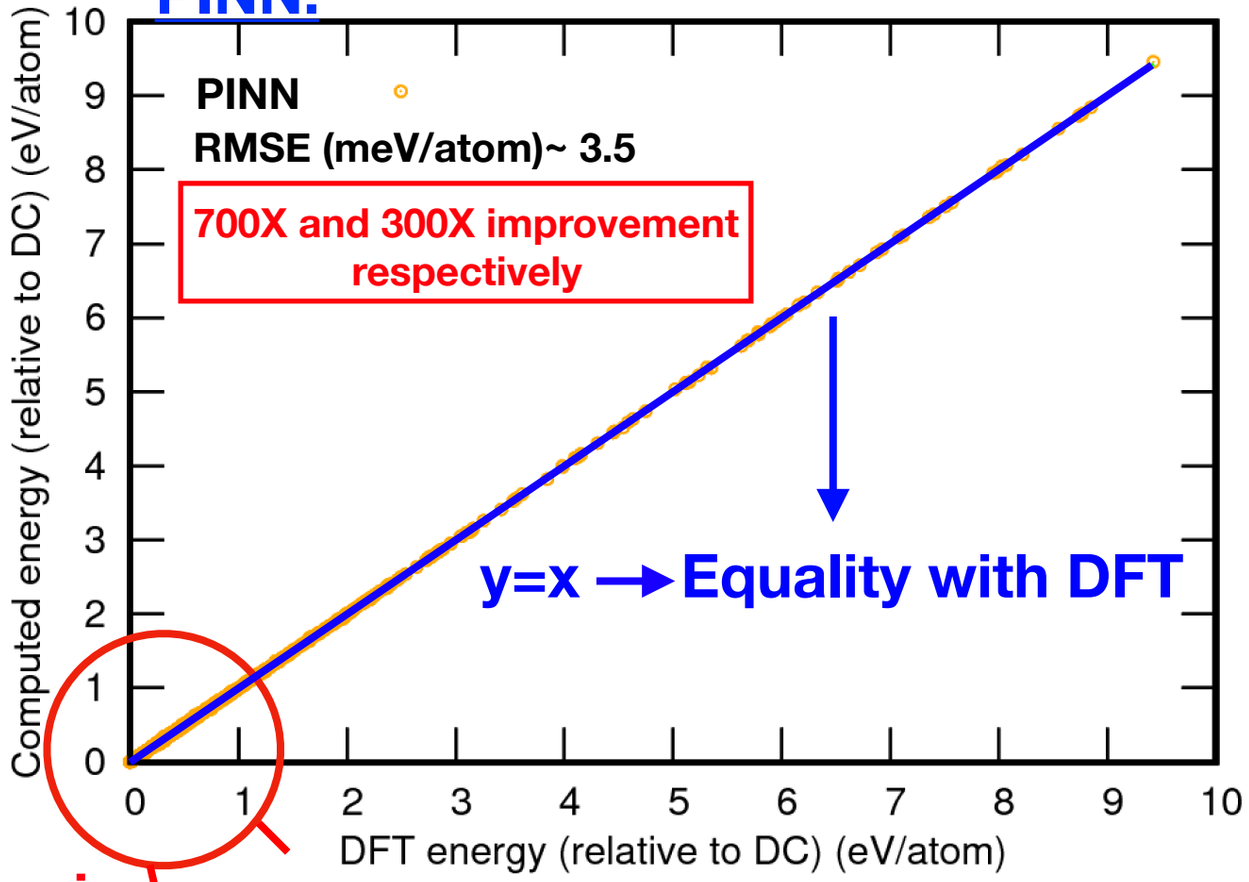
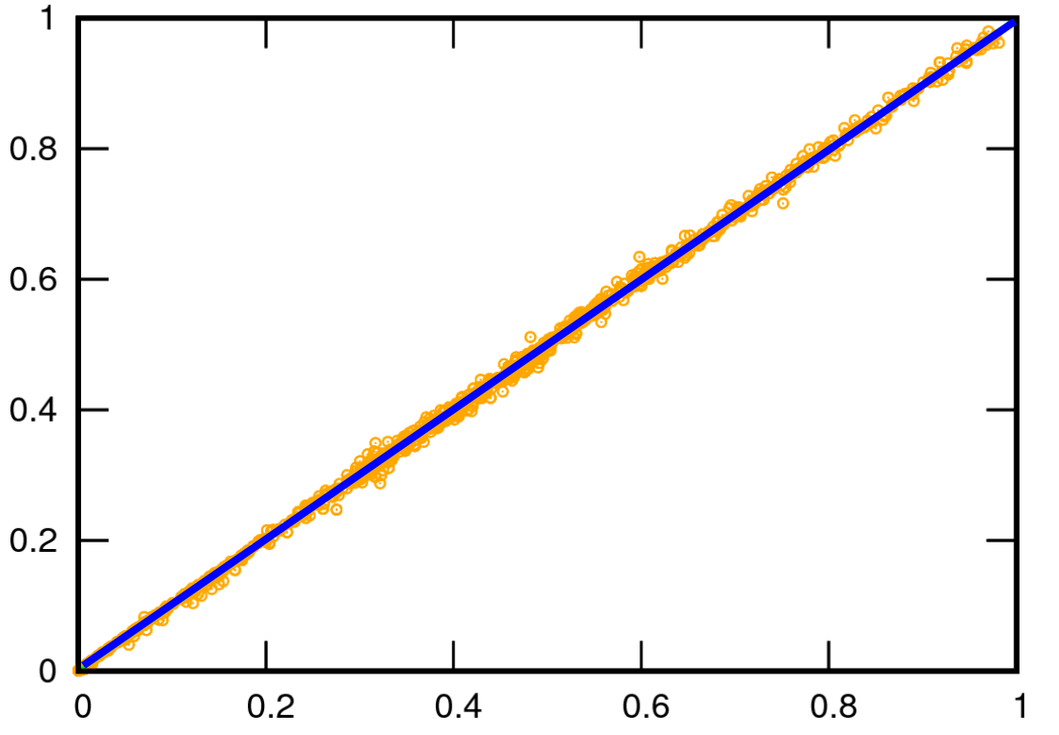
Si PINN comparison with traditional potential

Traditional potentials:

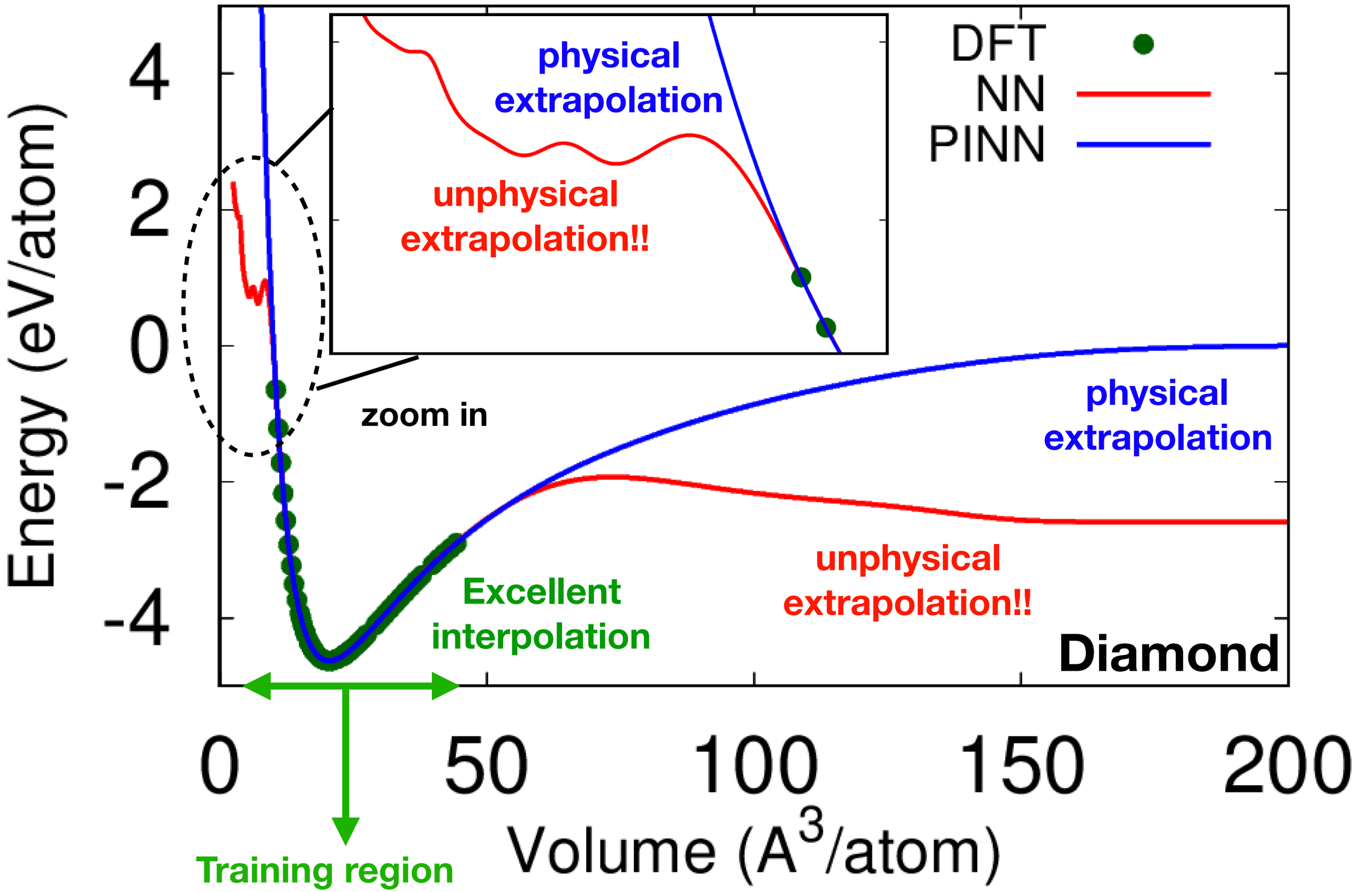


PINN:

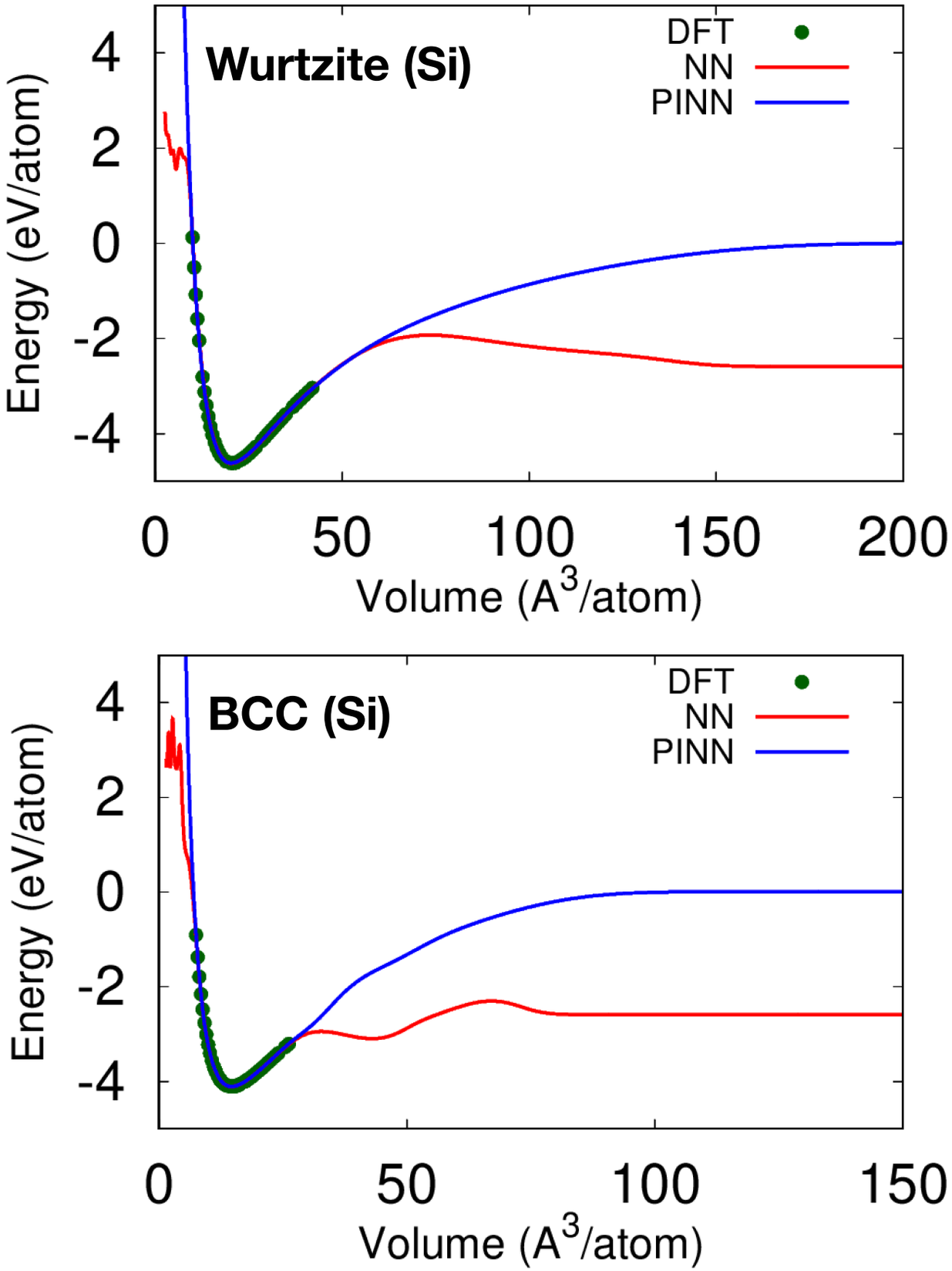


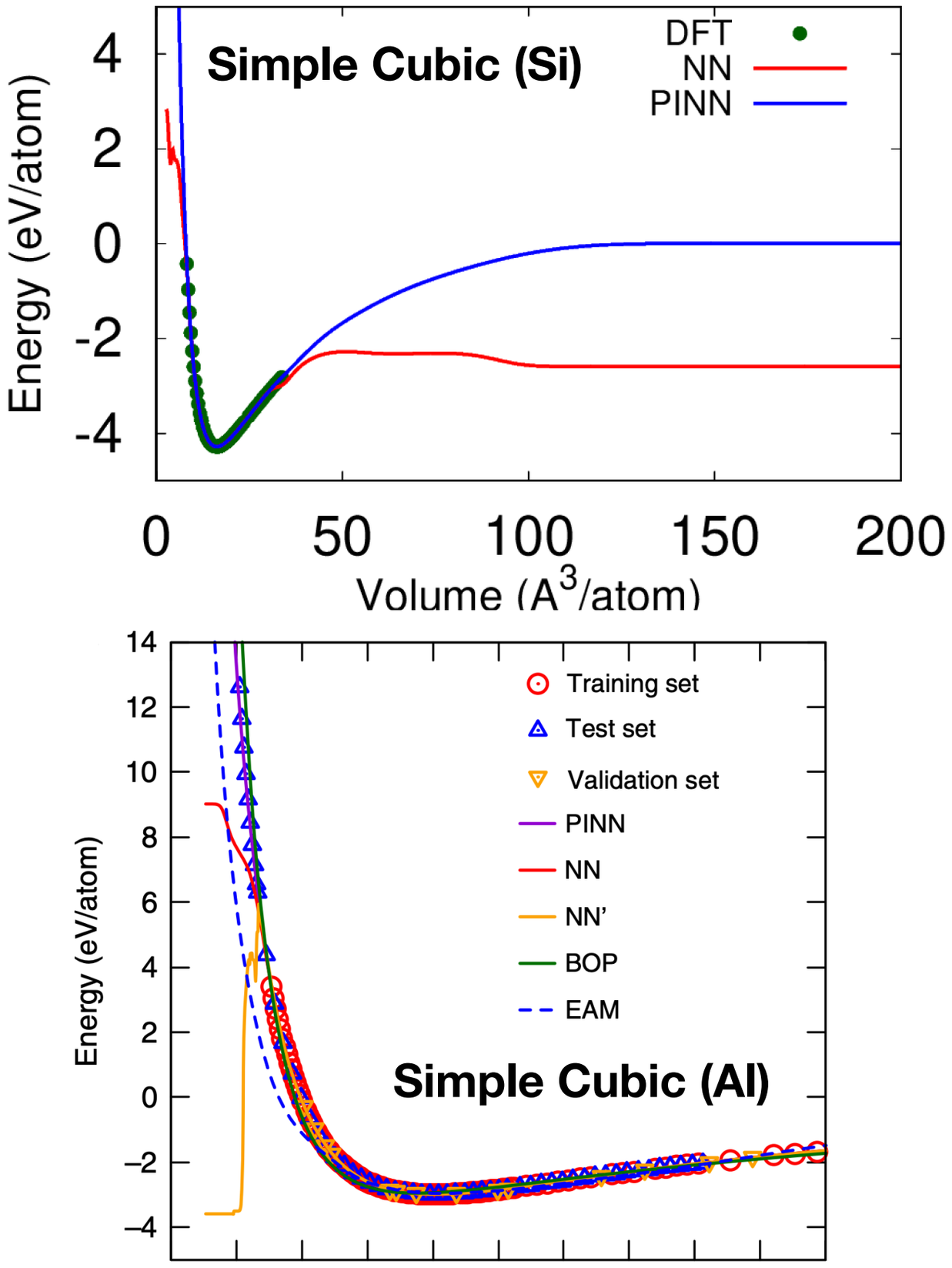


ANN vs PINN Extrapolation

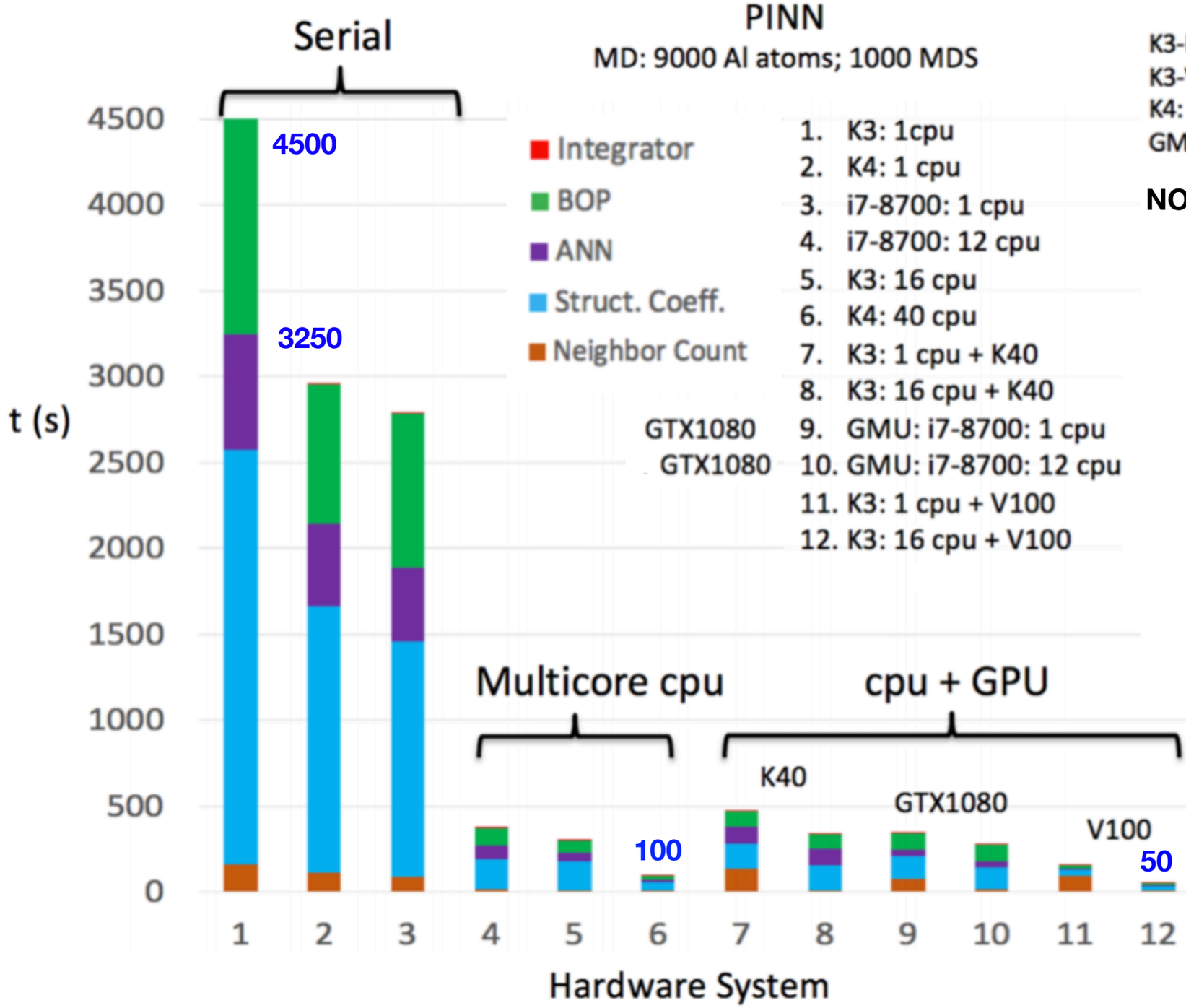


ANN vs PINN Extrapolation





Computational efficient



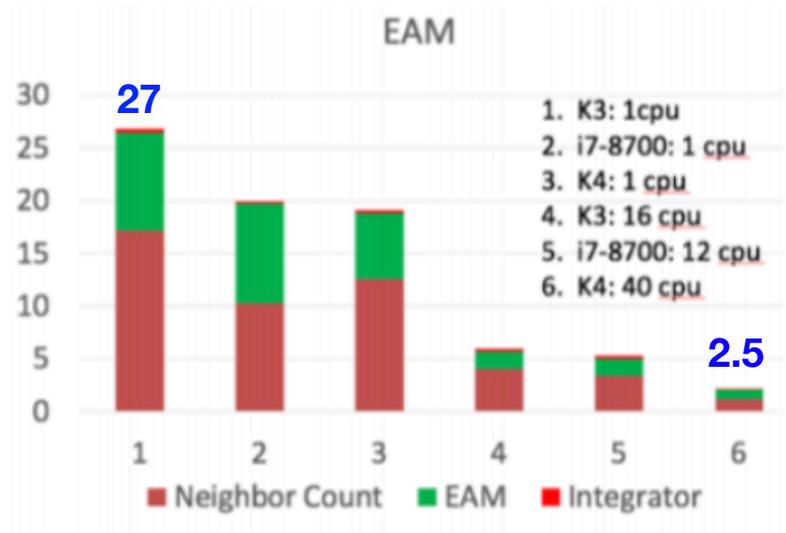
1. K3: 1cpu
2. K4: 1 cpu
3. i7-8700: 1 cpu
4. i7-8700: 12 cpu
5. K3: 16 cpu
6. K4: 40 cpu
7. K3: 1 cpu + K40
8. K3: 16 cpu + K40
9. GMU: i7-8700: 1 cpu
10. GMU: i7-8700: 12 cpu
11. K3: 1 cpu + V100
12. K3: 16 cpu + V100

GTX1080

GTX1080

K3-K40: SGI ICE Altix X 16 core cpu + NVidia Kepler K40 GPU
K3-V100: SGI ICE Altix X 16 core cpu + NVidia Volta V100 GPU
K4: Intel 6148 Skylake 40 core cpu
GMU: Intel i7-8700 CPU 12 core cpu + NVidia GTX1080 GPU

NOTE: results sensitive to hyper parameter choice



PINN vs EAM

serial: 166X slower
40 CPU: ~40X slower
GPU: ~20X slower

NN vs EAM

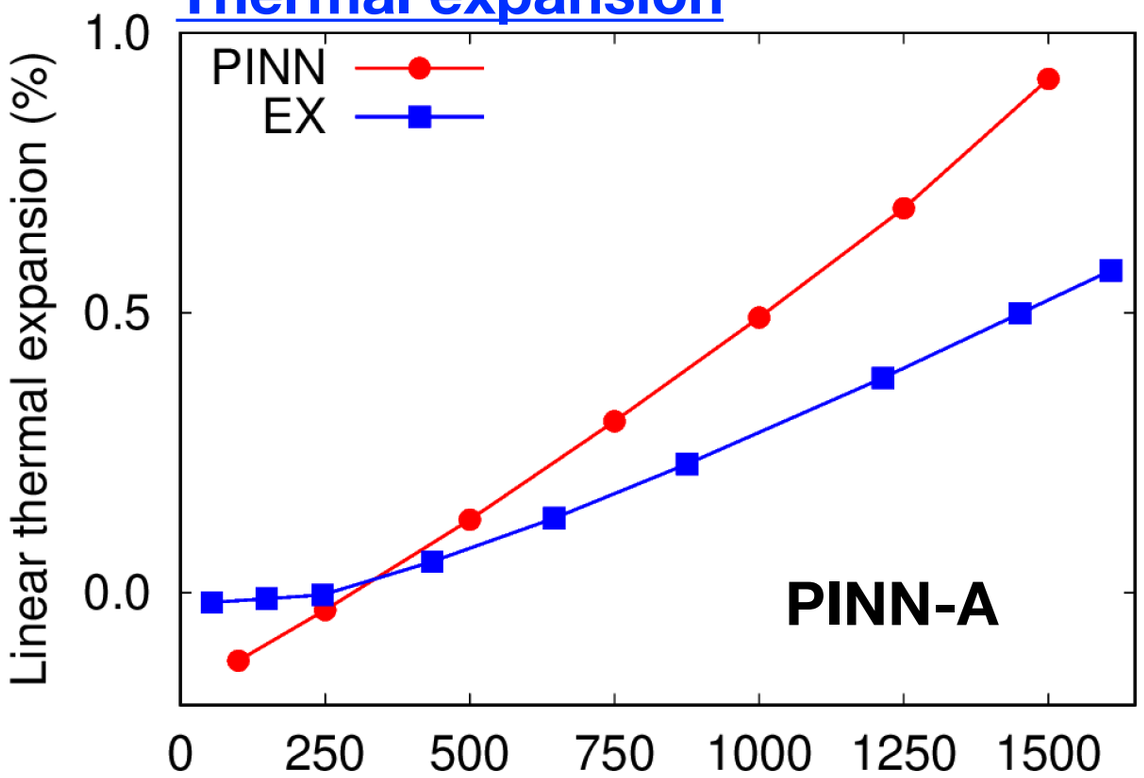
serial: 120X slower
40 CPU: ~30X slower
GPU: ~15X slower

Source: Vesselin Yamakov (NASA)

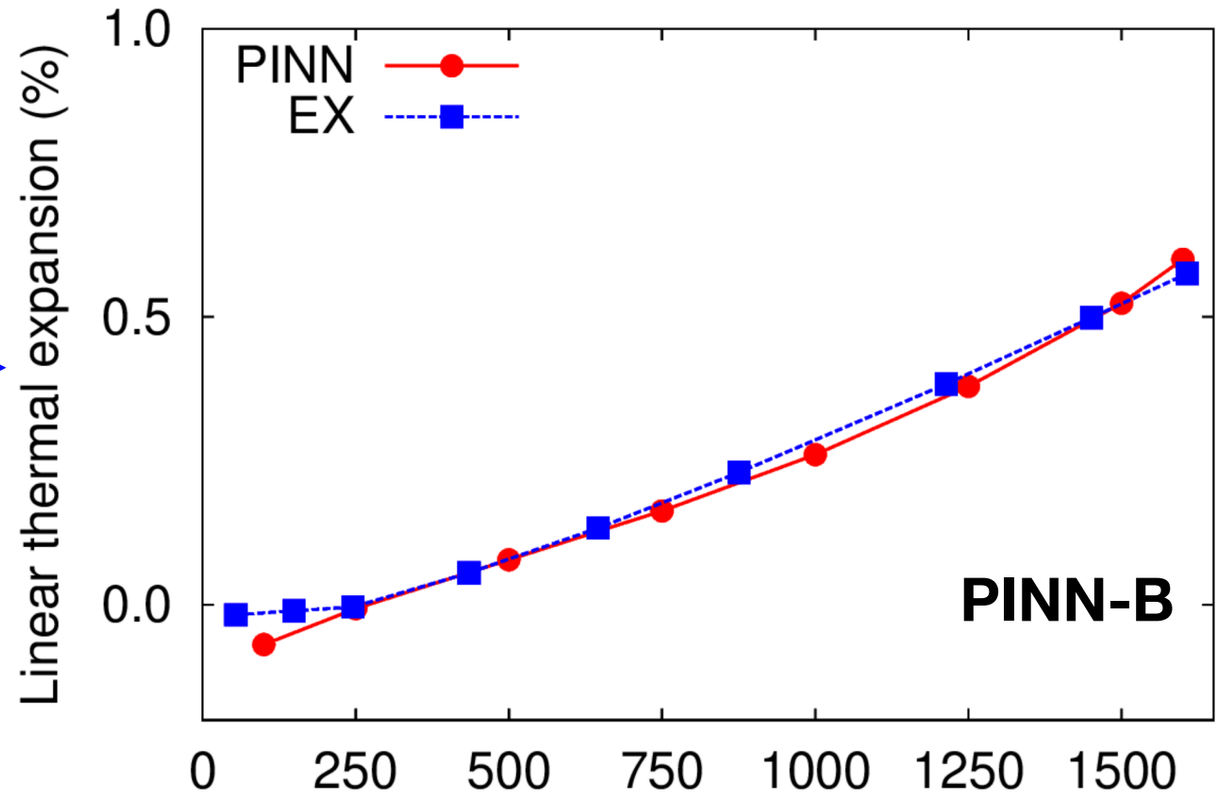
Paragrand MC:https://software.nasa.gov/software/LAR-18773-1

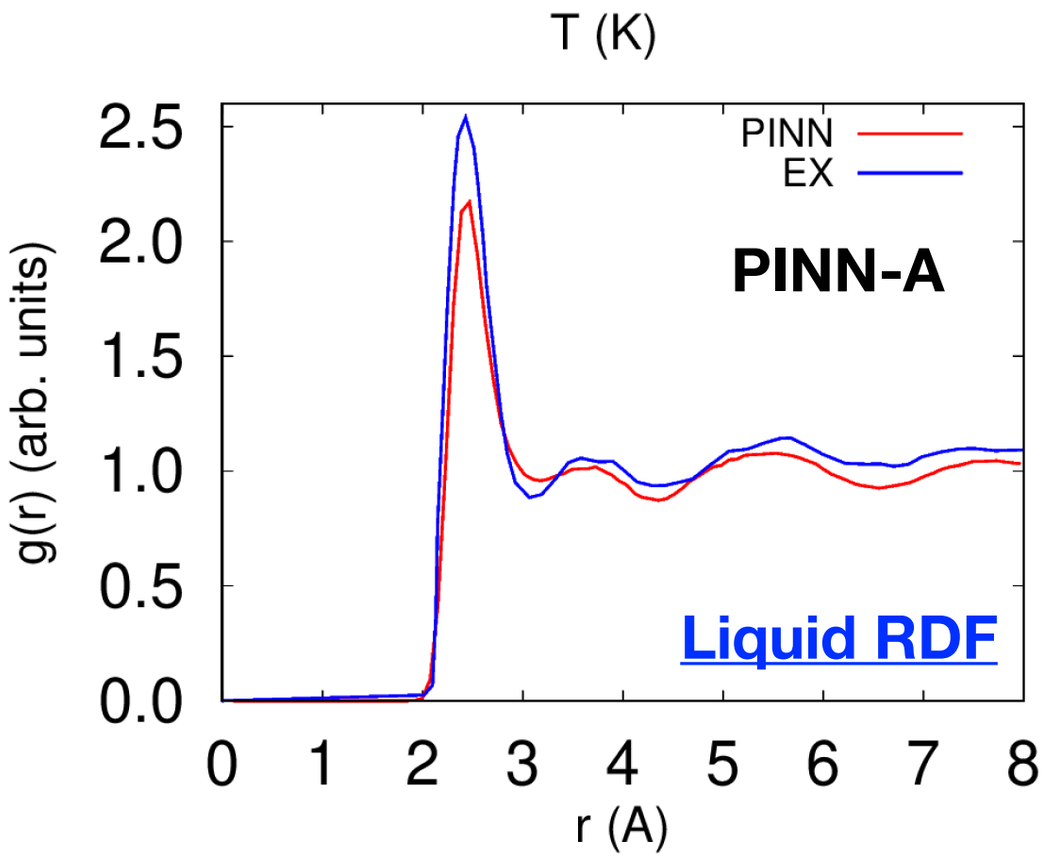
Thermal properties (preliminary)

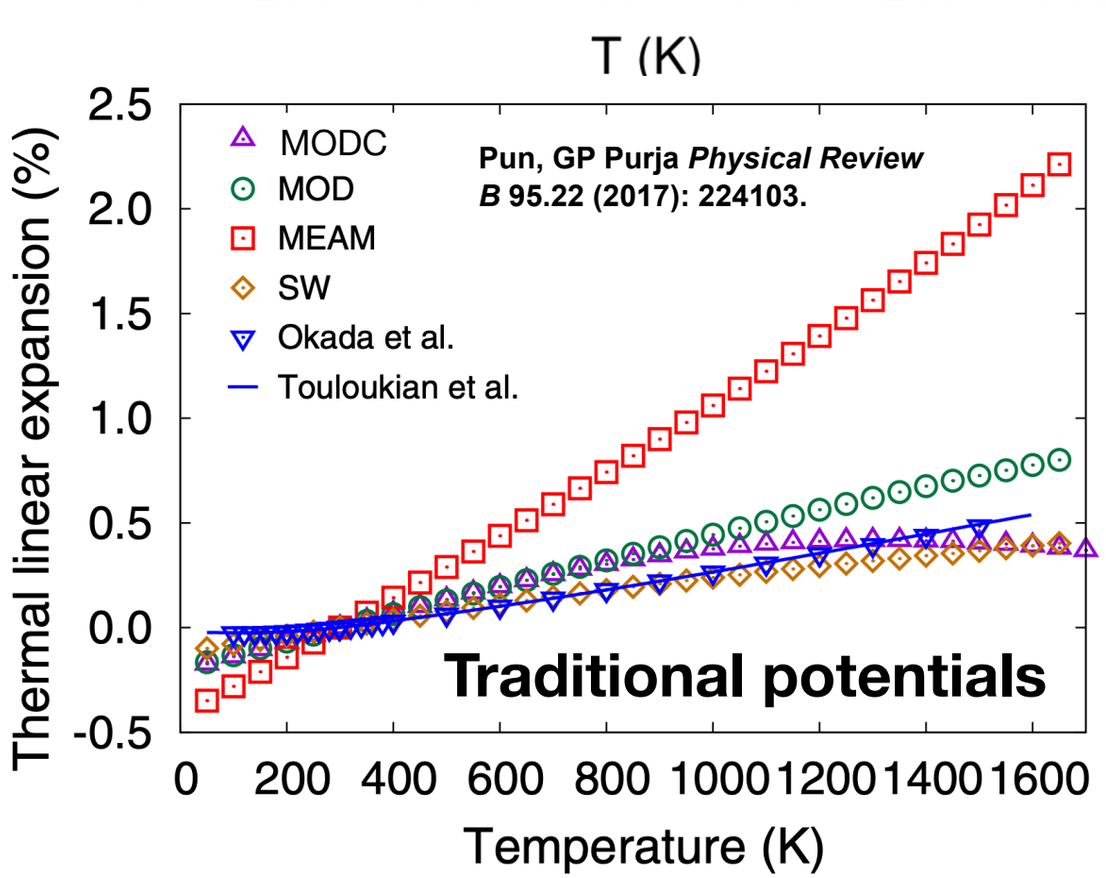
Thermal expansion



systematic improvement →







Future work

- Get PINN_BOP working in LAMMPS
- Hyper-parameter tune (speed/accuracy)
- Explore other Chemical systems:
  - Ge, Pt, Cu
- Binary: SiGe, SiAl, …. etc
- Possibly explore other traditional potentials formats
  - (PINN_EAM, PINN_ADP, etc)
- Applications
  - study thermal properties of 2D structures
    - Si ,Ge, SiGe

Conclusions

- Developed a new silicon interatomic potential using the new PINN potential format
- Even in preliminary stage we are obtaining excellent agreement with the DFT energies
- Current potential reproduces DFT data around ~500x better than current traditional potentials
- Better transferability than ANN potentials
- Investigating methodological considerations to streamlining the fitting procedure for faster future development

Acknowledgements

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- Yuri Mishin
- Adam Robinson
- GMU,NRC,NIST

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