Locating favorable point defects with active learning

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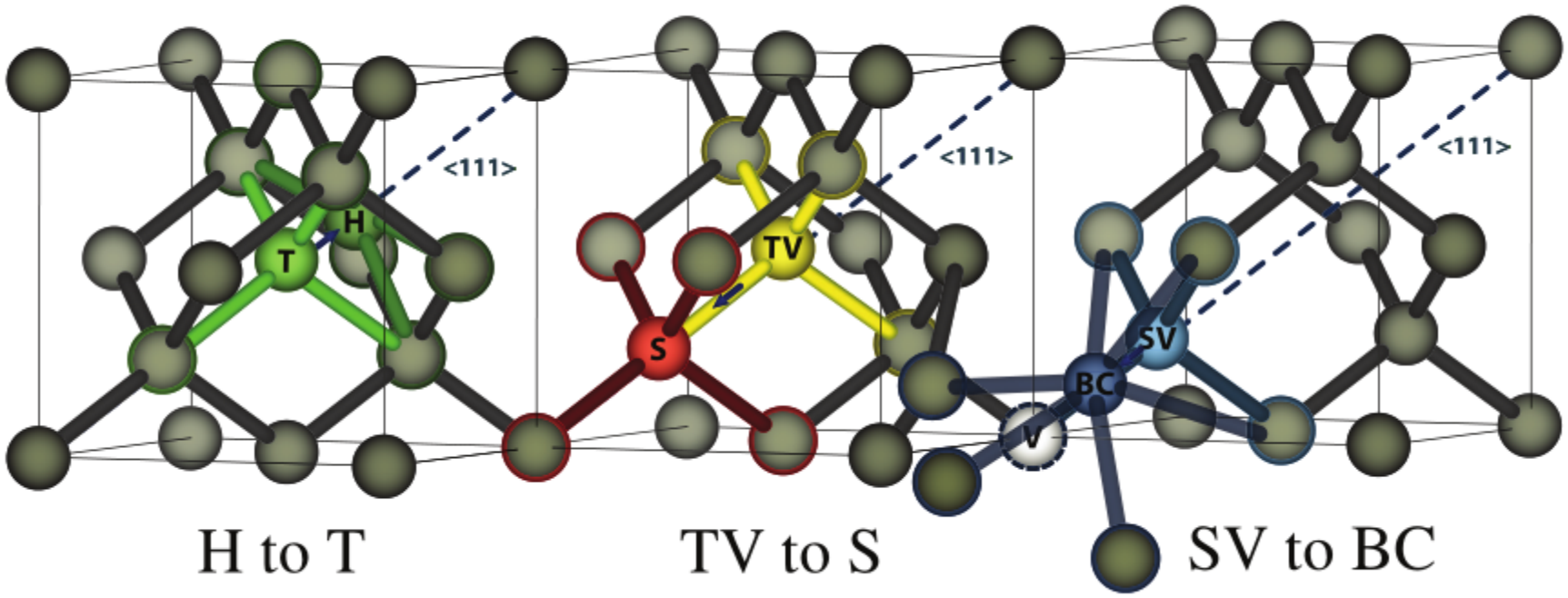
Defect control in Si

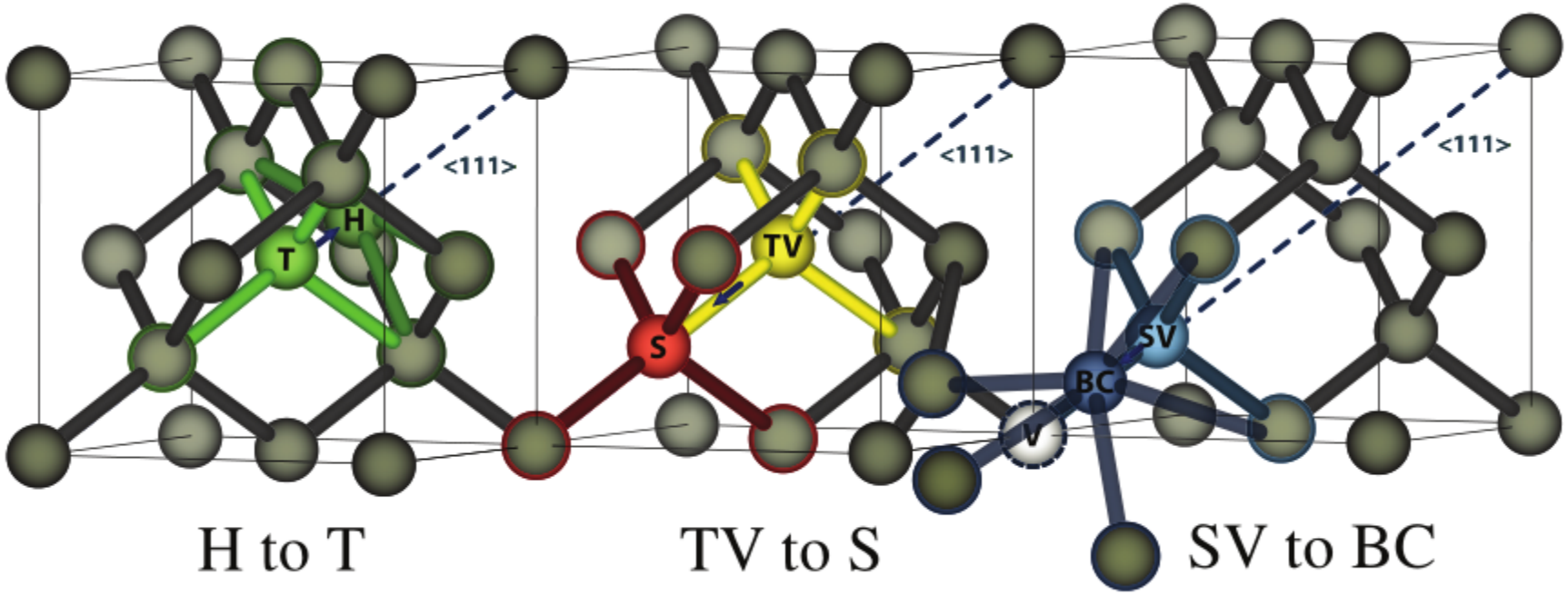
Control defects by understanding their nanoscale behavior

Defect positions



Defects are often atomic point defects

High-throughput screening

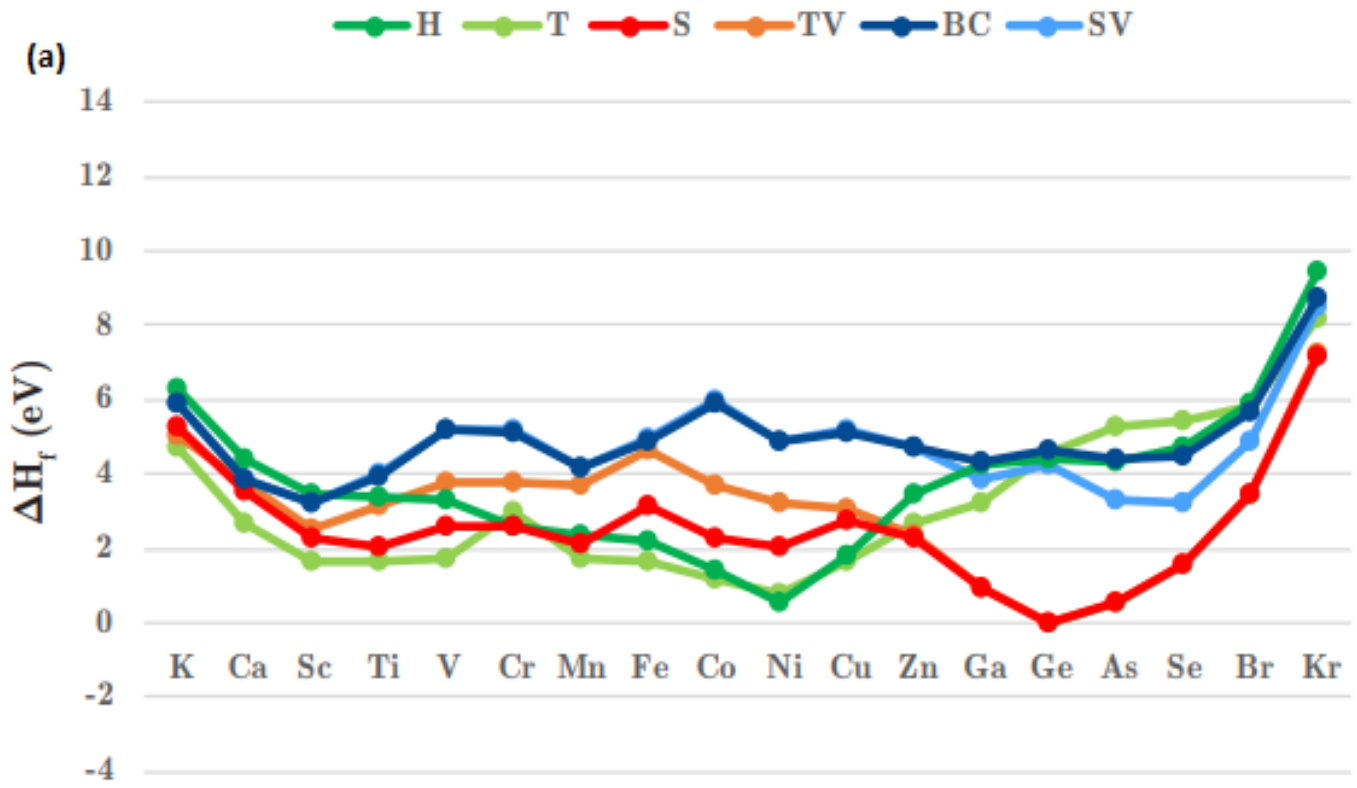


Number of systems to simulate:

6 defects·72 dopants·2 materials ·2 methods = 1728

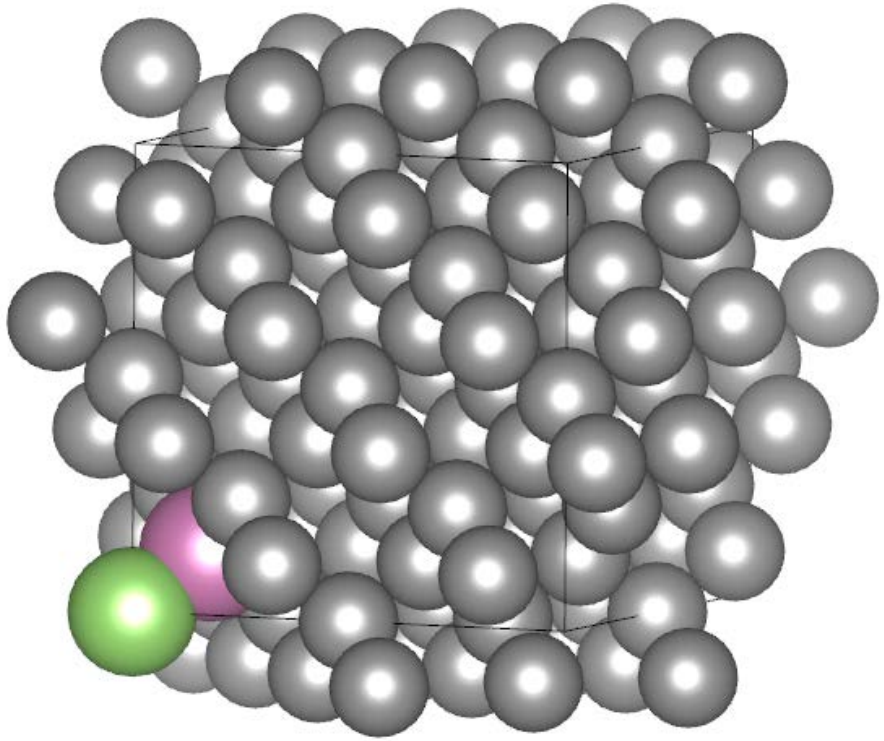
Results

Period 4 in Si



Results are smooth, do we need to simulate everything?

Problem: look for likely substitutional pairs



Even at near distances: 72 · 72/2 = 2592 combinations

Find ones with lower energy

Predict results using gaussian process

Fits an ensemble

Uncertainty can be used to decide where to sample next

Active Learning

Generate training data for the predictive model

DFT simulation

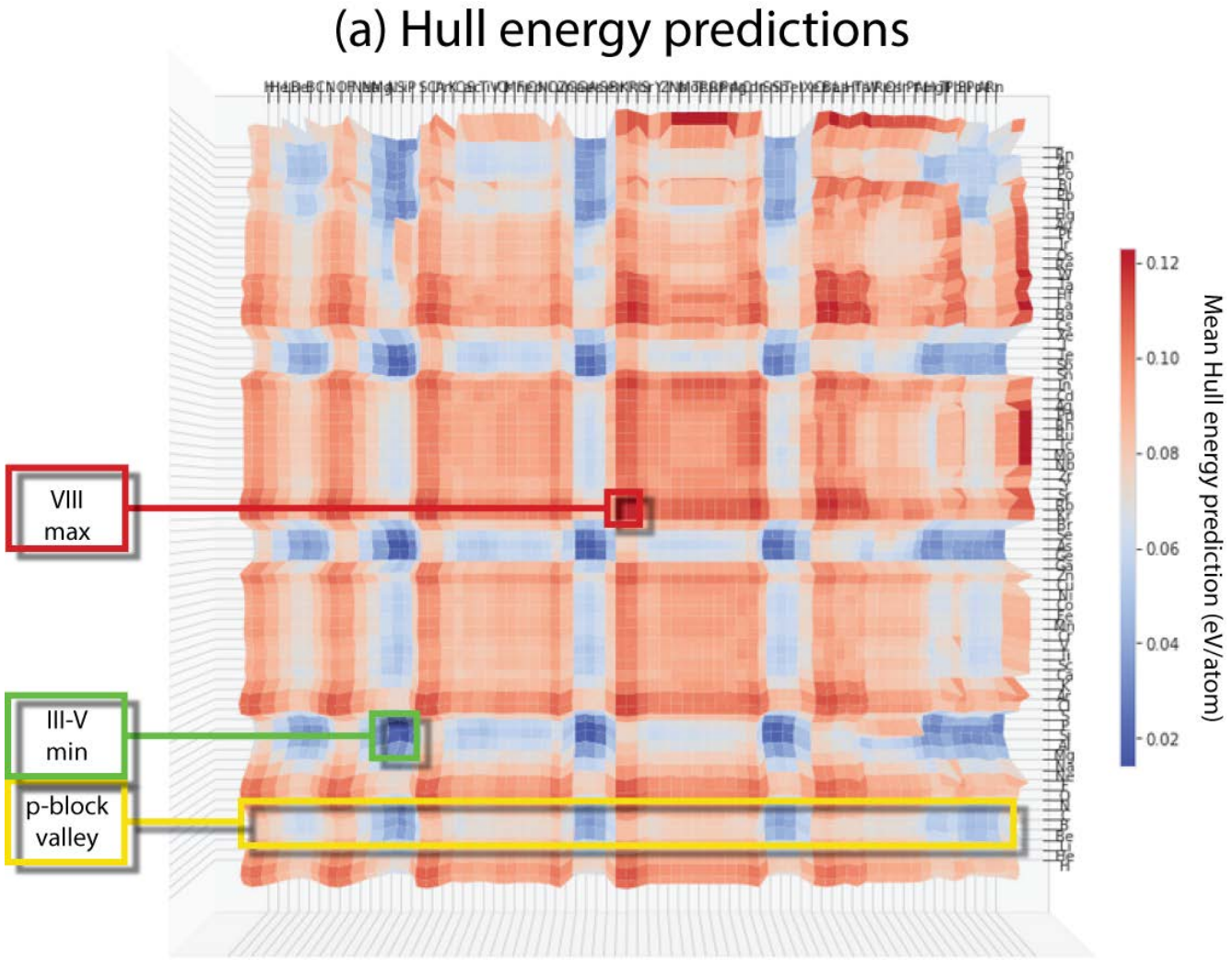
Gaussian process

DFT result

Mean, stddev

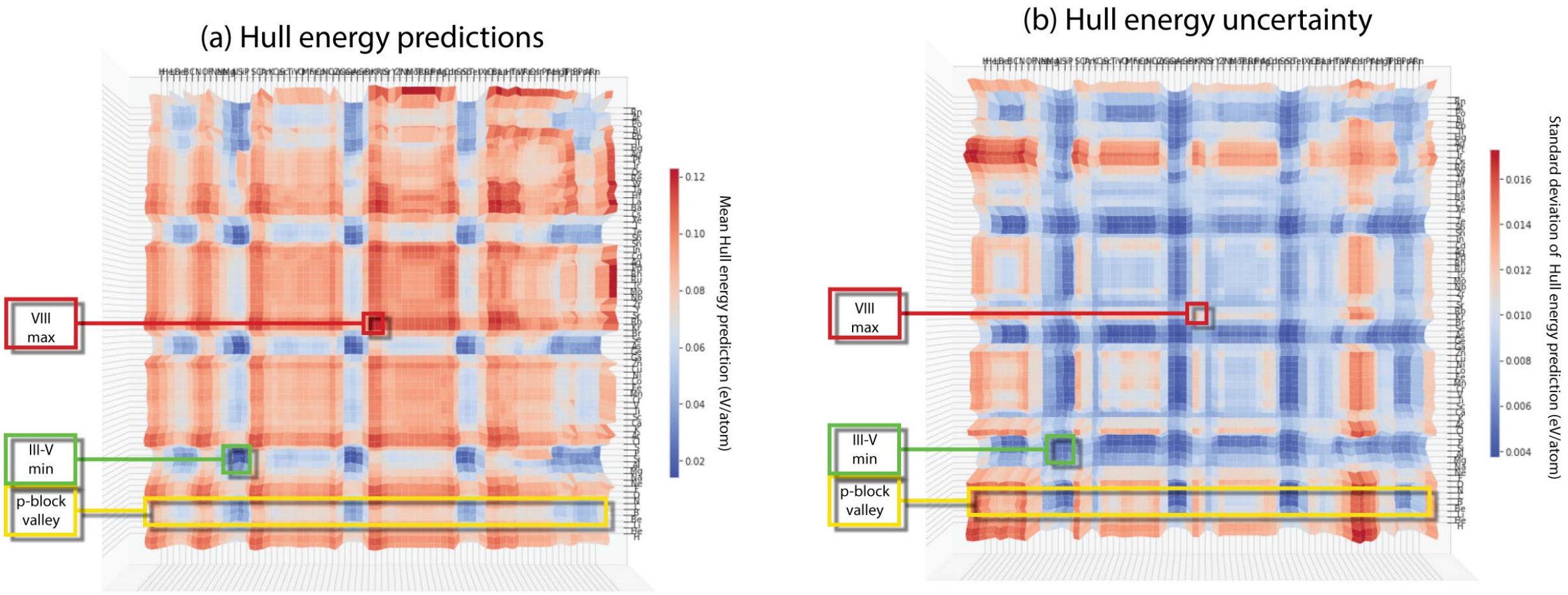
Given prediction and uncertainty, which defect is most interesting?

Gaussian process predictions



10% of calculations already gives a very good overview

Gaussian process predictions



The model is most certain in the lowest energy regions

The problem

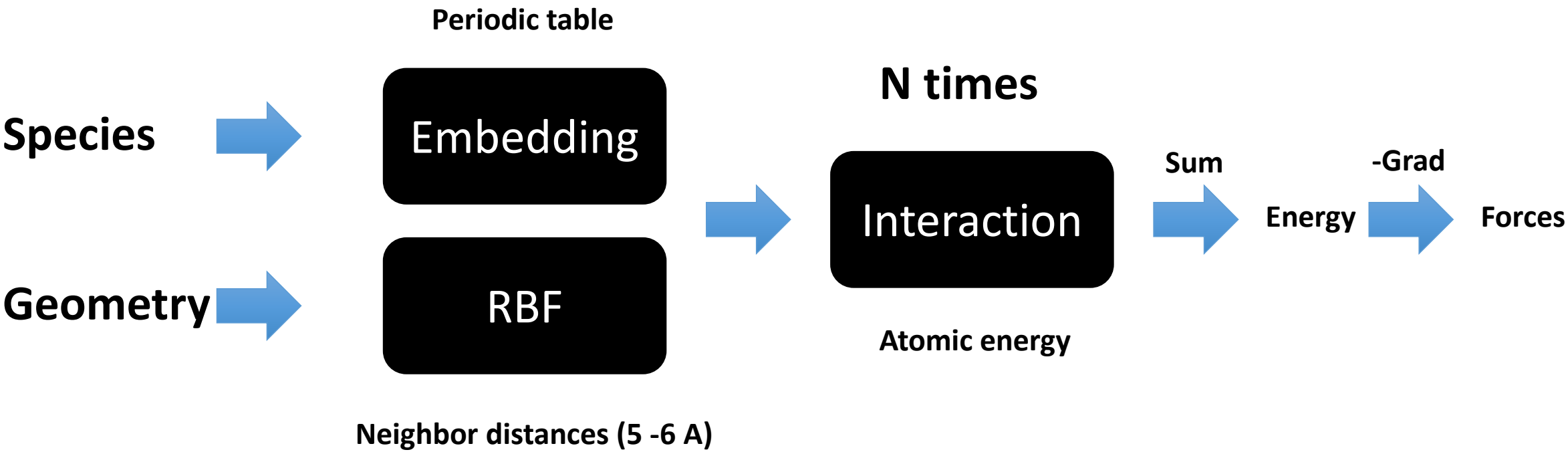
How do we get to more realistic systems:

- **High temperatures: many configurations, requires MD**
- **Interacting and diffusing defects**

Need complex models, able to process large amounts of geometric data

Deep learning

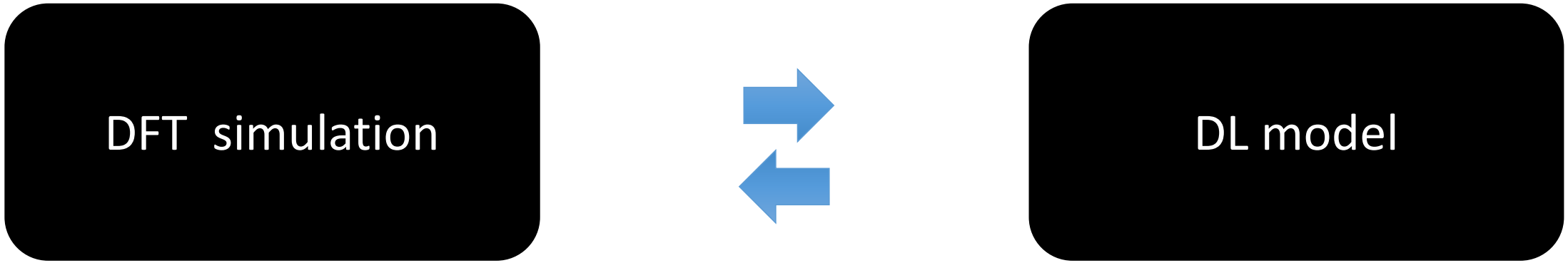
Geometric models: deep learning



SchNet architecture can fit a smooth potential energy surface

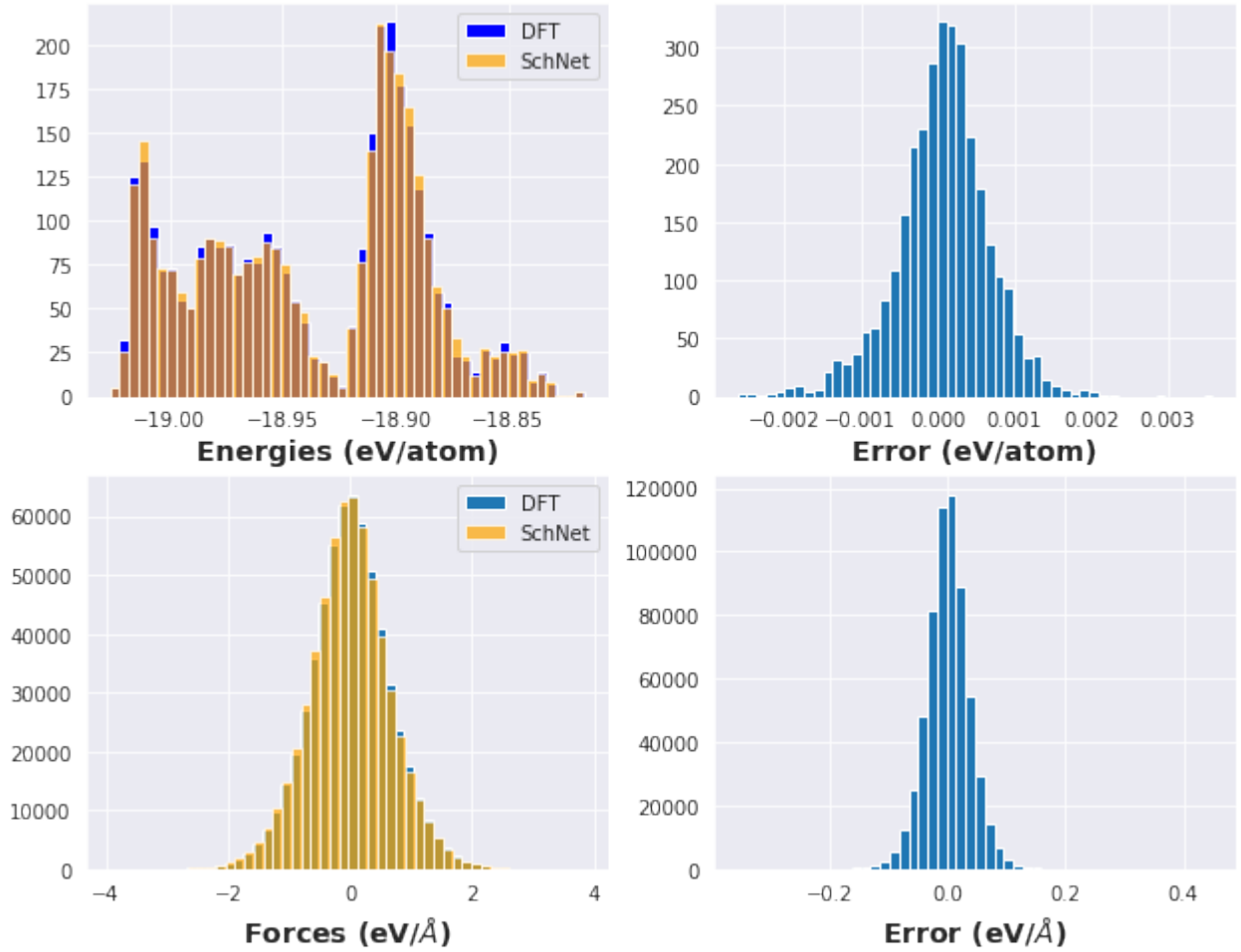
Fit to ab initio MD

Active Learning



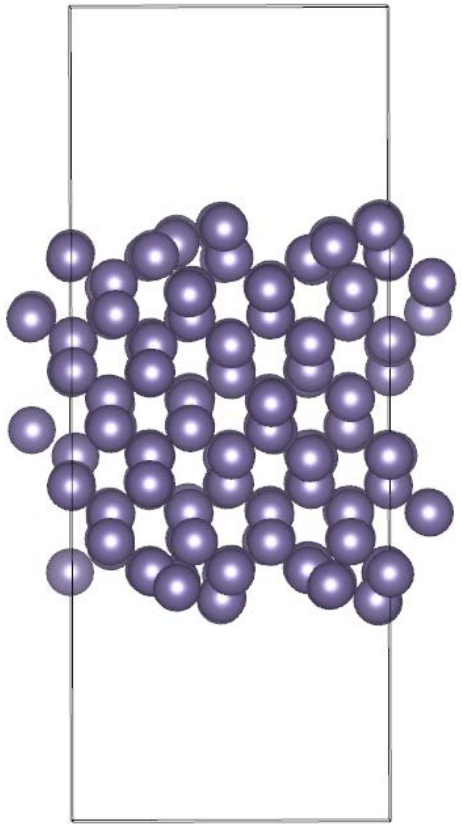
Need two ingredients: good predictions and reliable ensembles

Bulk and vacancy in a 64 atom Ge cell

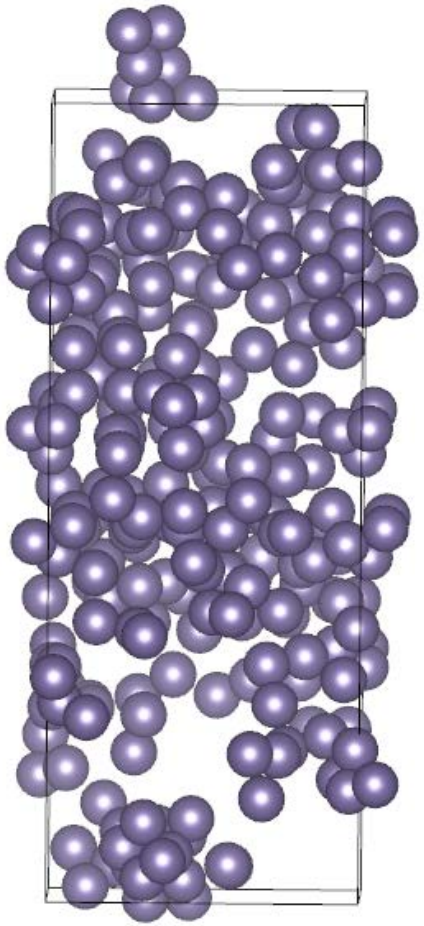


Isolated point defects can be fit well also for high T

Illustrating the energy scale

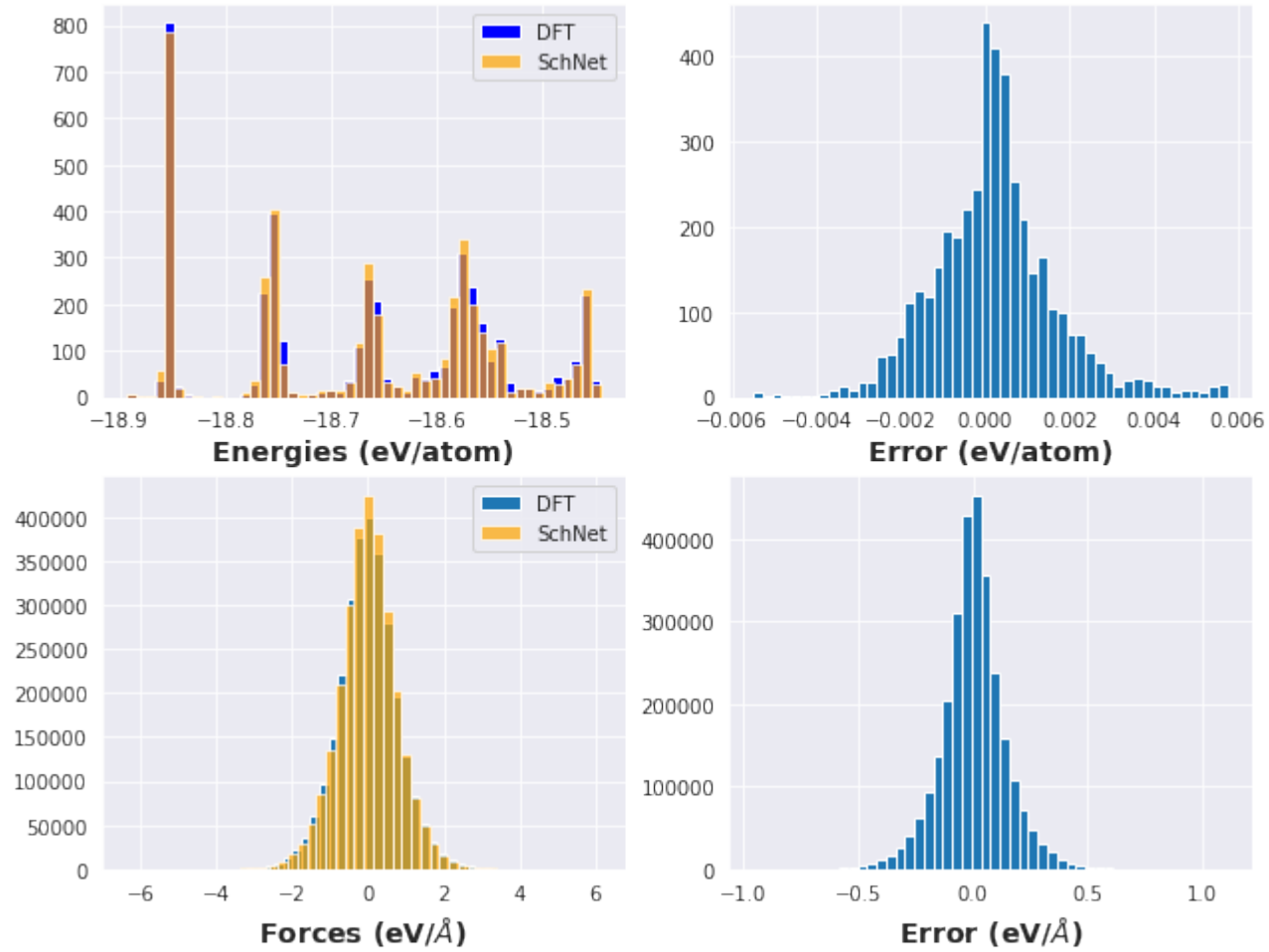


-18.84 eV/atom



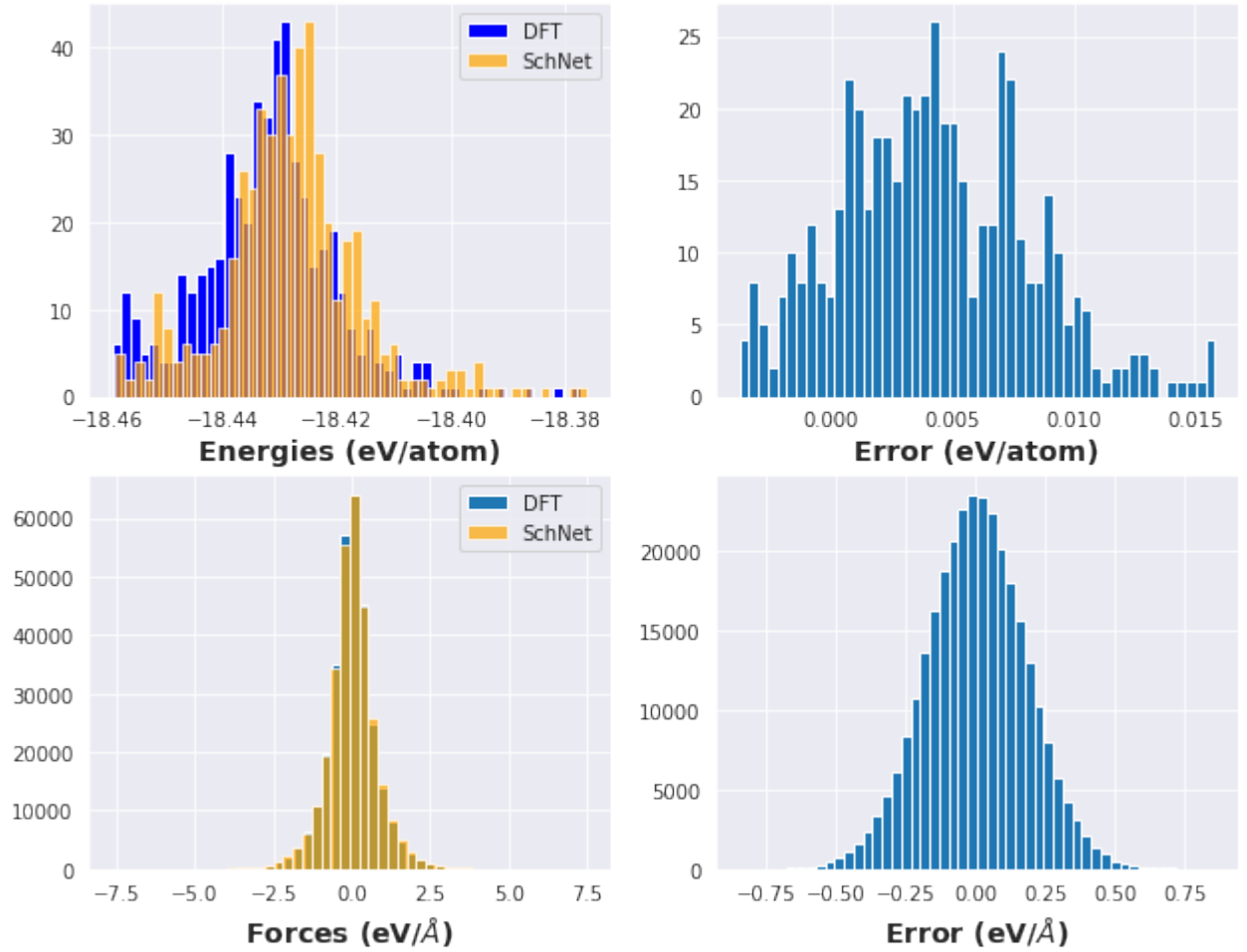
-17.9 eV/atom

111 surface with 224 atoms with T up to 2000 K



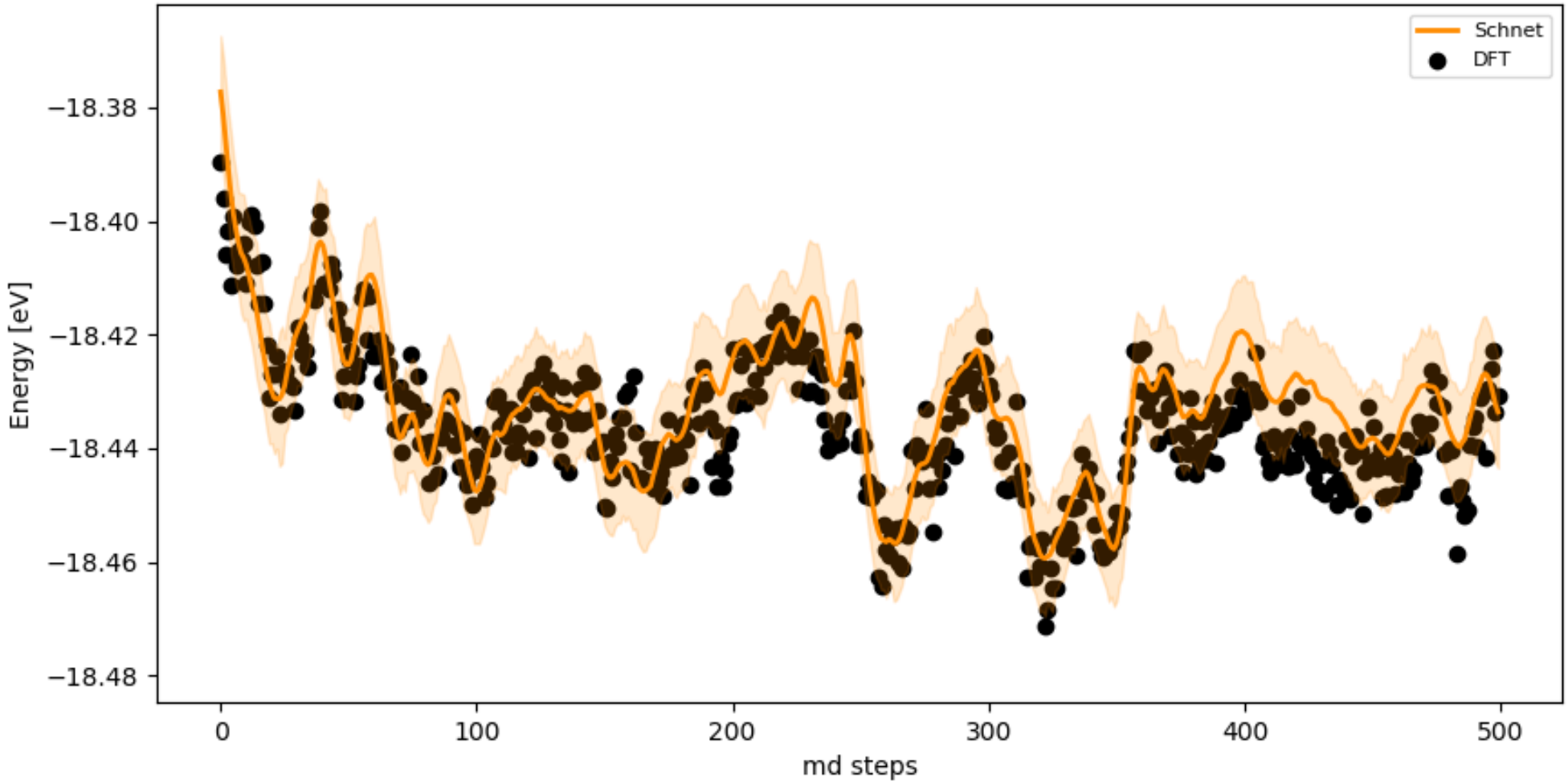
Data up to 2000K, energy okay, forces more difficult

13 vacancies in 216 atoms



Training data only includes interactions of up to 3 vacancies

What about uncertainties?

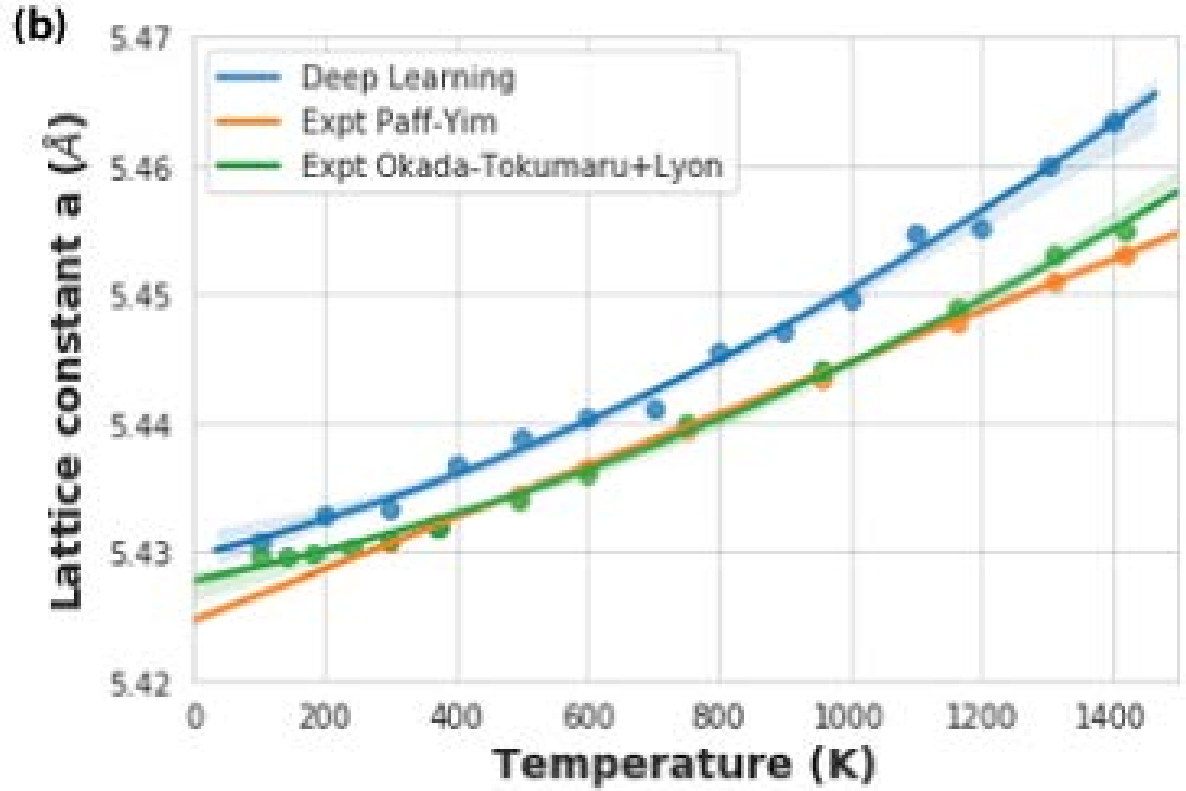


The key challenge is to generate reliable ensembles with limited compute

Conclusions

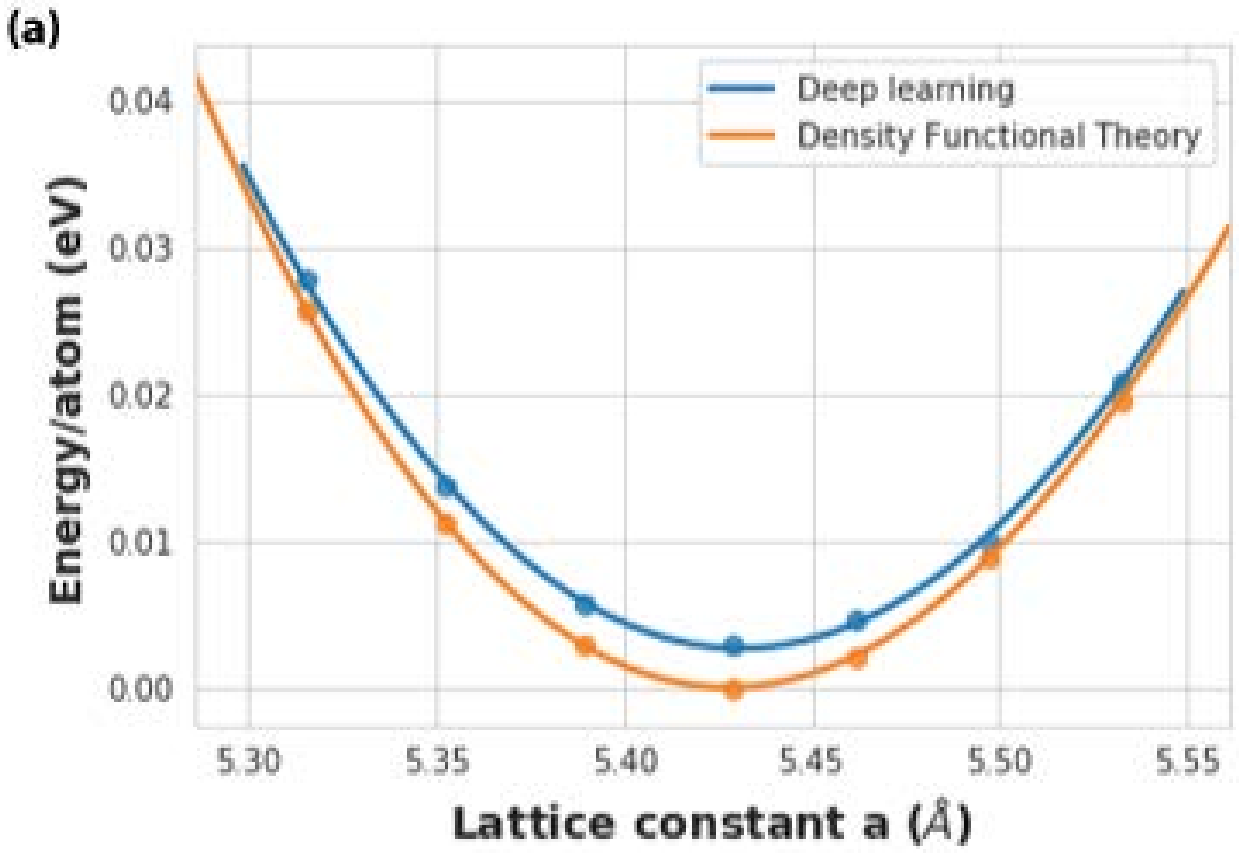
- Study of defects is important in many solid-state applications
- Active learning can greatly increase the speed of screening
- Deep learning models can handle defect dynamics given enough data
- Reliable and fast uncertainties for deep learning models remain a challenge

SchNet results 2: Molecular Dynamics Si



Thermal expansion good till 1000 K, constant offset (speedup 5k)

SchNet results 1: Si EOS



DFT:

- **a = 5.428 Å**
- **B = 99.69 GPa**

Schnet:

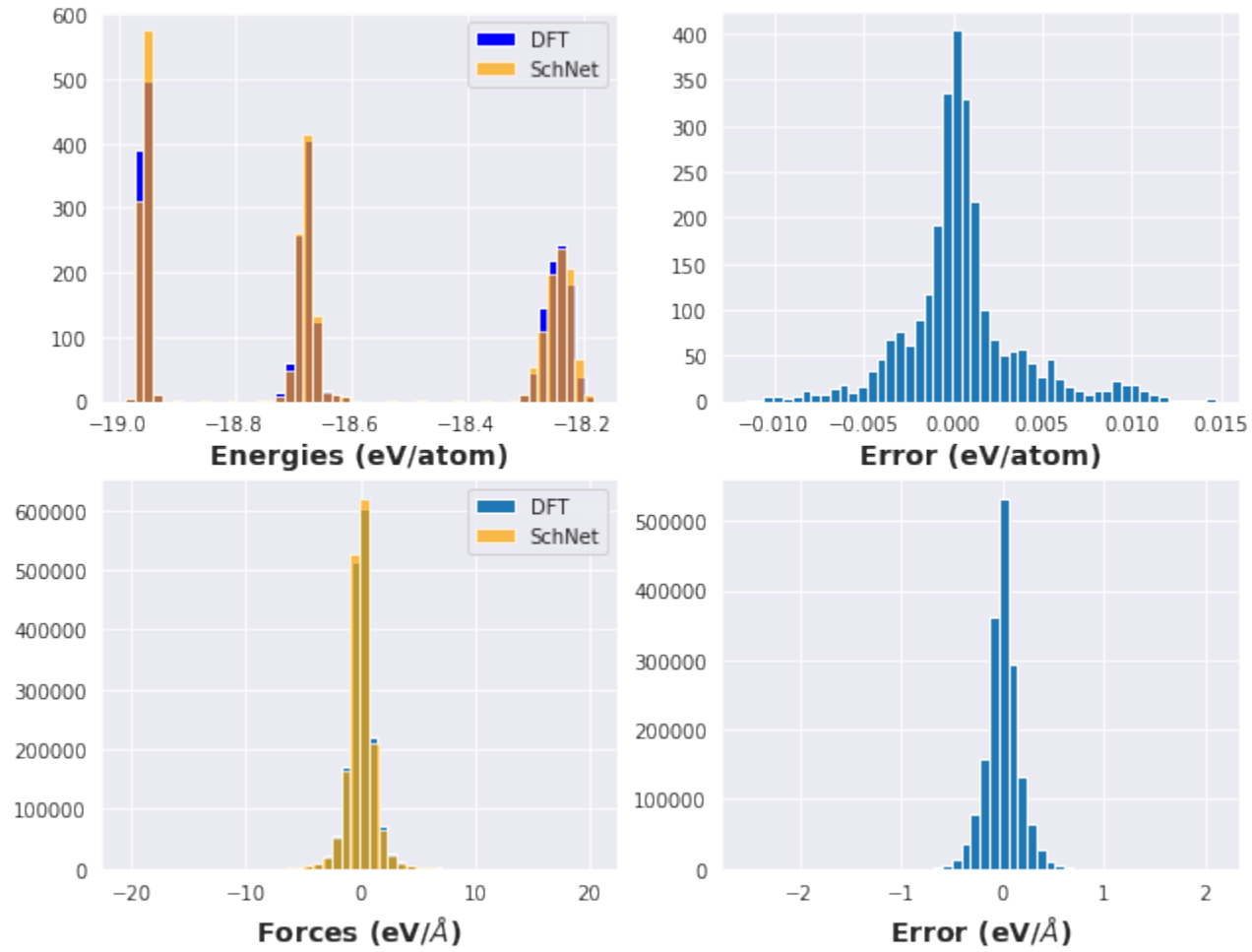
- **a = 5.430 Å**
- **B = 94.52 GPa**

Experiment

- **a = 5.43 Å**
- **B = 98.8 GPa**

Error on energy of 3 meV/at is comparable to that of DFT

3 Vacancies in 216 atoms



More complex situations require more data