Chapter 8: Machine learning techniques in nanoscale energy transport
Section 8.3: Machine learning based nanostructure optimization

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Convergence during training is monitored by validating NN results over another independent set called “testing set.”

NN is able to capture the physics!
Once trained, the NN can be quickly used to evaluate $k$ of many structures, which would be impossible using MD only.

Next step: check using MD simulation if the NN predicted lowest $k$ is indeed correct.

If **yes**, then optimal RML is found. If **no**, then put that data in training set and retrain the NN.
Another case study:

- **Problem statement**: Find structure with minimum/maximum Interfacial Thermal Conductance (ITC)

- **Solution method**: Bayesian Global Optimization (BGO)

Bayesian Global Optimization

- The principle:
  - Calculated the ITCs of n candidates in the design space
  - How to choose the next candidate for the next simulation?

![Diagram showing the mapping process](image)

- Using the learned regression function, predict the ITC of other candidates, and choose the one which is expected to be best
- Calculate ITC of new structure, and add it to the dataset. Now the dataset contains n+1 simulations.
Machine learning based structure optimization

- Results obtained for a small system, 8 atomic layers (12870 candidates)
- All optimizations converged within 438 computations (3.4% of total candidates)