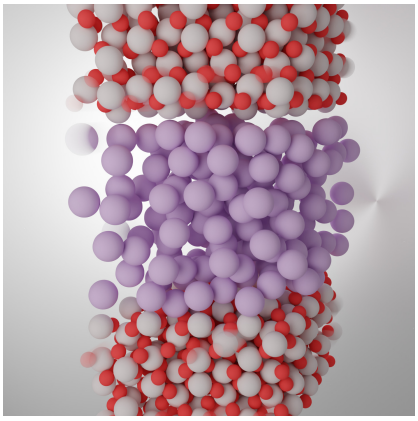
Training of Machine-Learned Potentials for phase change materials

The group of Prof. Salinga at the Institute of Materials Physics focuses on the study of materials for novel neuromorphic computing hardware. So-called phase change materials (PCMs) offer a large electrical and optical property contrast between crystalline and amorphous states, which are desirable properties for applications both in electronic and photonic memory and computing applications.

For decades, atomistic simulations have contributed significantly to our understanding of structure and properties of these materials. While calculations based on Density Functional Theory (DFT) provide very high accuracy, they typically limit the simulation of atomic dynamics to systems of less than a thousand atoms over less than a nanosecond in time.

Today, Machine-Learned Potentials (MLPs) offer an attractive combination of the accuracy of DFT simulations with the efficiency of classical potentials. This allows for accurate simulations of the dynamics on an atomic scale for systems of many thousands of atoms over tens of nanoseconds. The MLP is trained on DFT calculations of as many and as different atomic configurations as possible, which remains a challenging task. This is particularly true for multi-component or interfacial systems.



Snapshot from the simulation of a thinfilm structure: Antimony (purple) sandwiched between an insulating oxide (grey/red). Atomic configurations like this are the basis for training MLPs.

Our group is now looking for highly motivated and committed students who, based on a large set of pre-existing structural data, will advance the training and usage of such MLPs in our group as a

Student assistant (5-10h/week).

We expect...

- interest in machine learning and atomistic simulations
- interest in working with a high performance computer
- personal initiative and high motivation

Your benefits

- Introduction to state-of-the-art computer-based methods in materials science
- Introduction to working in a high-performance computing environment, with possible applications in all areas of science and engineering
- Collaboration in a young, dynamic team

Have we attracted your interest?
Then contact Prof. Salinga (martin.salinga@uni-muenster.de).