Title

Master project: Atomistic modeling for new generation nanoelectronics - optimizing interatomic interactions with Bayesian inference and machine learning

Description and objectives

The concept of 3D heterogeneous integration in nanodevices is defining the future of nanoelectronics while creating all sorts of challenges associated with new kinds of heterogeneous interfaces. Large-scale atomistic simulations with millions or even billions of atoms running on the best supercomputers in the world are commonly required to tackle such challenges, defining one of the core expertise of our Modeling&Simulations group at Empa (https://www.empa.ch/web/s204/modeling-simulations). The accurate and efficient atomistic modeling of thermodynamics, mechanics, heat and mass transport in nanocomposite materials and at heterogeneous interfaces requires the optimization of interatomic interactions to experimental and first-principles calculations. In this project, you will learn to use Bayesian inference and machine learning methods to solve such optimization problems for one of the industry-relevant nanocomposite materials. The optimized interatomic potential will be then applied to deepen our understanding of selected material at elevated temperatures and in presence of internal and external stresses. All the modeling results will be then verified experimentally by our collaborators at Empa, with the possibility for a student to participate in such activities (optional). This project would lead to the successful completion of the Master's thesis and a follow-up scientific publication, acting as proof of your new skills relevant for both academia and industry.

Workplan

The general workplan is defined in the description. The final project will be tuned to the skills and interests of the student.

Required skills

The applicants should be familiar with one and interested in learning the basics of the other methods:

1) Gaussian processes and machine learning,
2) Bayesian inference and Markov chain Monte Carlo
3) Molecular dynamics simulations and first principles (DFT) calculations

The project requires good knowledge and prior experience with the corresponding Python tools. Prior experience with LAMMPS would be an advantage.

Languages

English (Advanced)

Location

Empa Thun

Remark

More internship and Master projects are available on our website:
https://www.empa.ch/web/s204/open-positions

For more details please contact Dr. Vladyslav Turlo vladyslav.turlo@empa.ch

Related masters

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Mechanical engineering	Mathematics
Microengineering	Applied mathematics
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Materials science and engineering	Physics
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