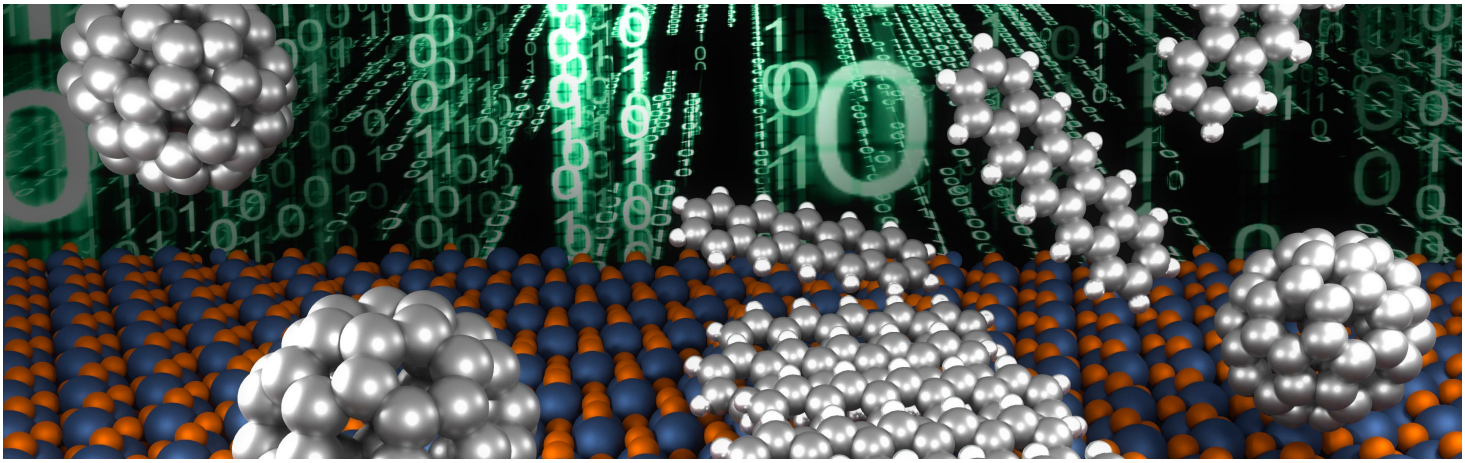
Artificial intelligence for materials physics
2020 Summer Project



Machine learning molecular surface layer formation with artificial intelligence

Project description

Would you like to experience the cutting edge of physics research?
Machine learning of quantum mechanics has become an exciting new research field. We teamed up with computer scientists to develop an original artificial intelligence (AI) approach for physics: you could use our Bayesian Optimisation for Structure Search (BOSS) tool for global optimisation, or work on big data materials analytics.

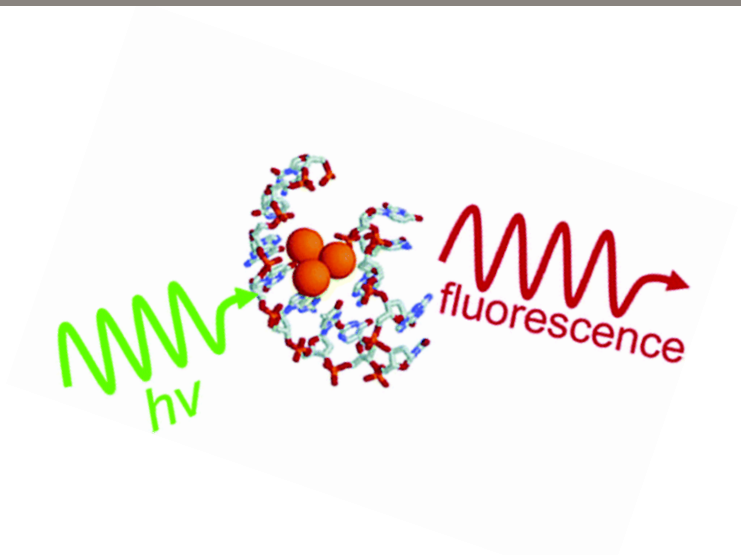
Do you enjoy programming and learning new coding tools?
Our Python codes require computational tests and gradient capabilities, but also applications on new problems. You would get hands-on AI experience and make movies and animations.

Uncover fundamental phenomena in physics with artificial intelligence!
You would use AI to design new advanced materials, guide experiments, or re-purpose materials for different functions and industrial technologies. In this summer project, you will be assisting experimental and computational groups at Aalto to make AI predictions based on their data. This project requires both programming skills and ideas on how to encode physics data efficiently for best AI results.

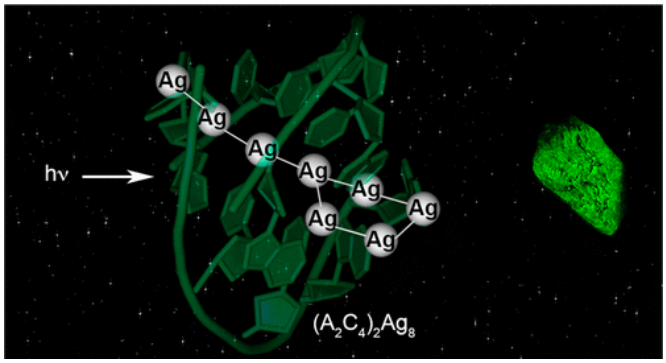
Computational Electronic Structure Theory (CEST) group
Project leaders: Prof. Patrick Rinke and Dr. Milica Todorović

Computational investigation of novel DNA-silver nanoclusters

2020 Summer Project



DNA-stabilized silver clusters (silver atoms shown in red) can have different fluorescent colours, which enable many bio-applications



First crystal structure reported for DNA-stabilized silver (Ag) clusters

Project description

Would you like to study novel materials with biological applications?

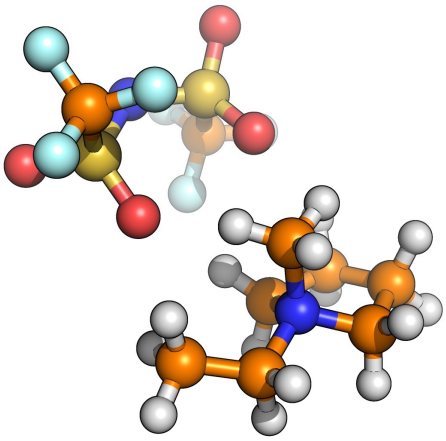
The DNA double helix is the pivotal biological structure for encoding genetic information in life. New DNA-based nanomaterials can be developed by integrating metal atoms into DNA. Such materials may have enhanced thermal stability, new physical and chemical properties, and diverse functionalities. In our group, we are mainly interested in DNA-stabilized silver clusters, which have unique DNA-sequence-dependent fluorescence. The high fluorescence quantum yields, good photo-stability, low toxicity, low synthesis costs, small cluster sizes and natural compatibility with DNA enable many exciting applications such as biosensor and bioimaging.

Are you interested in cutting-edge computational materials science?

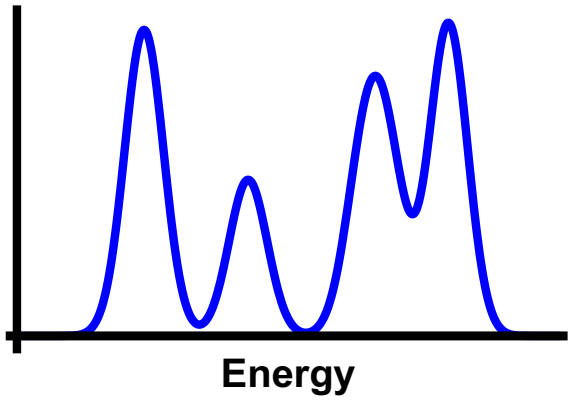
DNA-stabilized Ag clusters have attracted much attention in recent years due to their potential applications. However, it is very challenging to obtain structural information for the clusters directly from experiment. Such structural information is required to understand cluster properties. In 2019, the first crystal structure of a new DNA-stabilized Ag cluster has been reported (right figure), which opens up new opportunities to study this novel material. In the project, you will build atomic models for DNA-stabilized metal clusters and explore their structural and electronic properties with computational simulations.

Computational Electronic Structure Theory (CEST) group
Project leaders: Prof. Patrick Rinke and Dr. Xi Chen

Quantum many-body physics for theoretical spectroscopy
2020 Summer Project



$$H|\Psi\rangle = E|\Psi\rangle$$



Structure **Computation** **Spectra**

Project description

Are you interested in quantum mechanics?

Quantum mechanics describes materials at the most fundamental level. With only the fundamental equations, we can predict material properties and design new materials for target applications. Understanding and predicting spectra, or how a material responds to external particles and fields, is essential for both fundamental science and improving performance in devices like photovoltaics.

Do you want to run calculations on supercomputers?

The equations are too difficult to solve with pen and paper. For this reason, we use high performance computing to numerically solve the problem. Our group develops state-of-the-art theory and computational packages to run numerical calculations on Finland's largest supercomputers.

We are seeking students with interest in running state-of-the-art quantum mechanical calculations to help benchmark new methods in quantum many-body physics. The students would run calculations on many hundreds or even thousands of CPUs and gain working knowledge of materials physics.

Computational Electronic Structure Theory (CEST) group
Project leaders: Prof. Patrick Rinke, Dr. Dorothea Golze, and Dr. Marc Dvorak