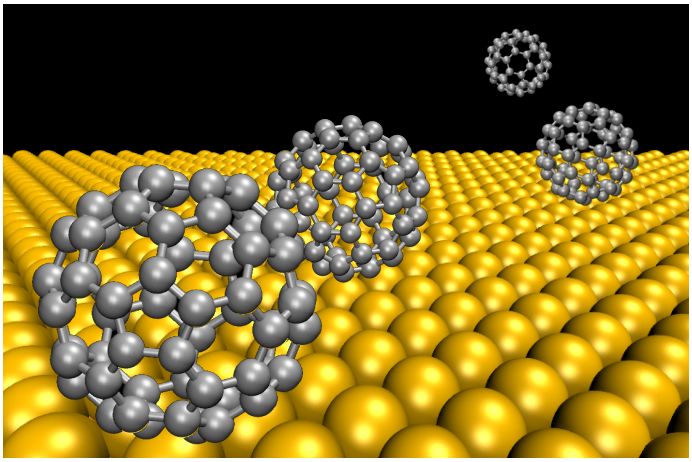
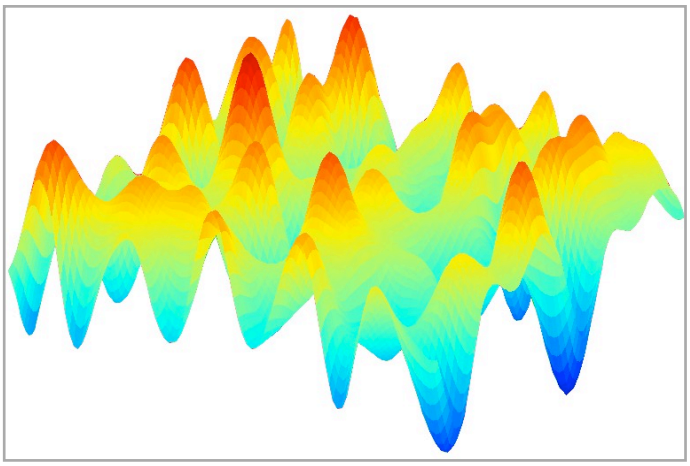
# Machine learning molecular self-assembly
# 2018 Summer Project



Fullerene molecules interacting on a surface



Machine learning a 2D energy landscape

## 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 machine learning approach for materials simulations: you will be using our computer code BOSS (Bayesian Optimisation Structure Search).

**Do you enjoy programming and learning new coding techniques?**

Our Python BOSS code needs better handling of atomistic symmetries and atomistic visualisation. You would extend BOSS capabilities and make movies and animations.

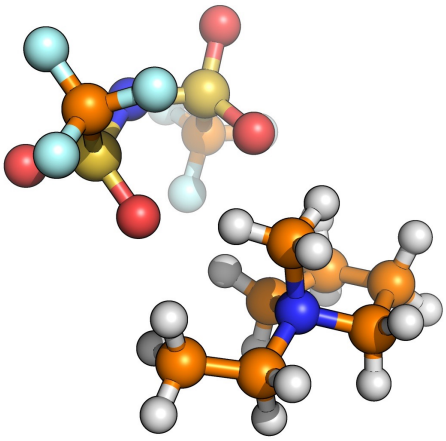
**Uncover fundamental phenomena in physics!**

You would apply BOSS to better understand the fundamental interactions of matter that are related to industrial technologies. In this summer project, you would investigate how fullerene molecules self-assemble on a metallic surface into molecular layers. This project is a collaboration with experimental partners who will perform the atomic scale experiments and imaging.

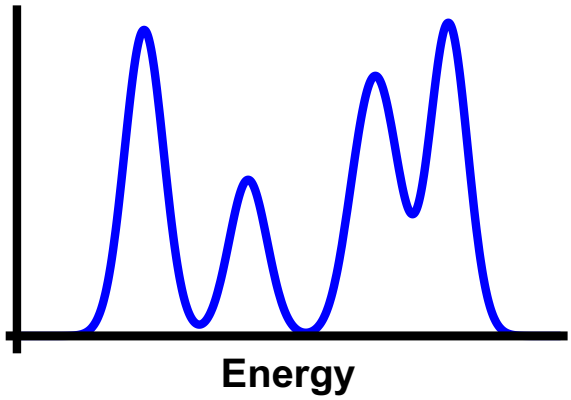
Computational Electronic Structure Theory (CEST) group
Project leaders: Prof. Patrick Rinke and Dr. Milica Todorović

# Quantum mechanical approach to machine learning of spectra

# 2018 Summer Project



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




**Structure** **Computation** **Spectra**

## Project description

**Are you interested in machine learning?**

Machine learning is a powerful new tool for understanding data - from facial recognition to playing Go, machine learning is popping up everywhere. Machine learning is becoming increasingly popular in physics and materials science where large data sets are available.

**Do you want to design materials for next-generation optoelectronics?**

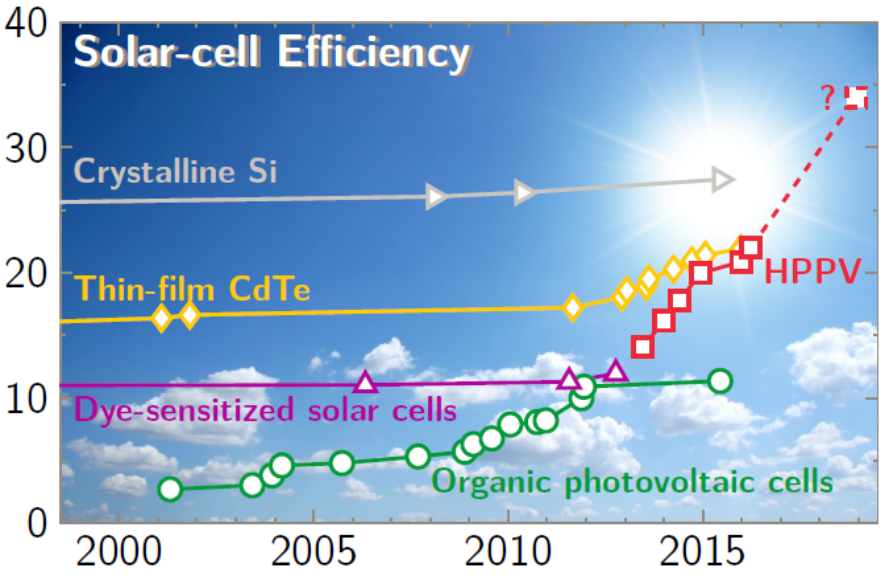
The performance of optoelectronic devices depends largely on spectral properties that are defined over a continuum of energies. Quantum mechanical calculations on supercomputers can predict these properties without the need to measure them in a laboratory, but the calculations come at a huge expense. One proposed solution is to train a computer to predict spectral properties without the expensive calculations. This is **machine learning for spectral properties.**

We are seeking one student with an interest in running state-of-the-art quantum mechanical calculations to help generate test data to train our under-development machine learning algorithm for spectral properties. This project is an opportunity to learn both machine learning basics and fundamental quantum mechanics.

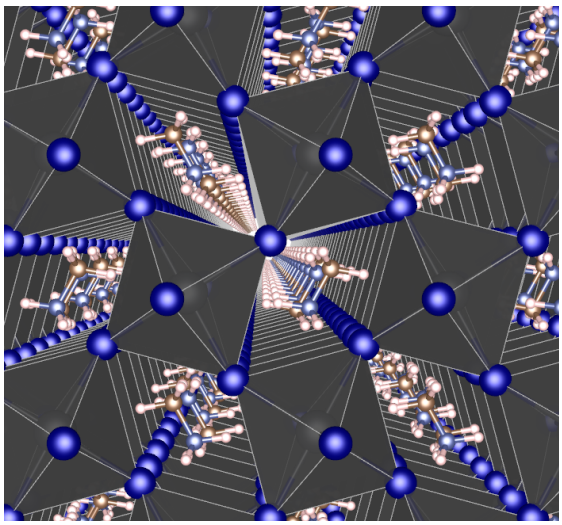
Computational Electronic Structure Theory (CEST) group
Project leaders: Prof. Patrick Rinke, Dr. Dorothea Golze, Dr. Marc Dvorak, and Annika Stuke

# Quantum mechanical exploration of novel photovoltaic materials

# 2018 Summer Project




solar cell efficiency evolution



structure of hybrid perovskite material

## Project description

**Would you like to participate in the solar revolution?**

Hybrid perovskites (HPs, right figure) are the rising star in emergent solar-cell technology. In only 5 years after their discovery, perovskite-based photovoltaic cells rose to record efficiency of ~22%, catching up conventional technologies such as crystalline Si or thin-film CdTe (left figure). Hybrid perovskites contain organic cations integrated within a metal-halide framework. They are cheap to produce from easy raw materials and promise affordable energy-conversion from the sun.

**Are you interested in cutting-edge computational materials science?**

To optimise the properties of HPs, we can vary the composition of the material by creating alloys of different metal and halogen atoms and organic molecules. This leads to a huge materials space, in which we need to find promising materials with desired properties. In this project, we will apply a materials discovery approach that combines quantum mechanical modelling with machine learning to efficiently scan the HP materials space. Our design criteria are high photovoltaic efficiency and high material's stability.

Computational Electronic Structure Theory (CEST) group
Project leaders: Prof. Patrick Rinke, and Dr. Jingrui Li