ETH zürich

Semester Project

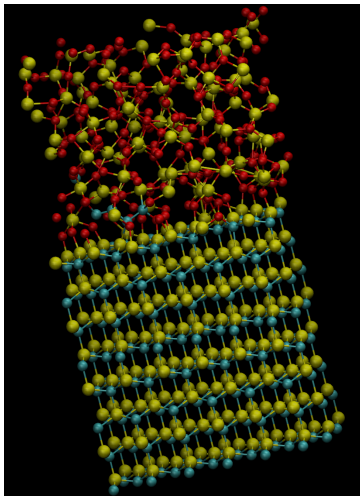
First-principles study of 4H-SiC/SiO_2 systems

Short Description
In this project the student will learn to use density functional theory and classical force fields to construct $4H-SiC/SiO_2$ structures. A particular focus will be on the formation of different types of defects and their properties. From these structures quantum transport simulations will be performed to extract relevant characteristics.

The Big Picture
Due to the growing energy consumption worldwide, energy efficiency plays an increasingly important role in our society. Electrical energy often has to be converted from AC to DC, DC to AC, as well as between frequencies and voltages. For these conversions often solid-state transformers, power inverters or rectifiers are used. Silicon has long been the material of choice for the channel of such devices. On the other hand, 4H-SiC, a wide bandgap material, seems to be a good alternative candidate because of its many advantageous properties.
However, 4H-SiC suffers from excessive electron scattering caused by defects at the $4H-SiC/SiO_2$ interface which lowers the channel mobility considerably. So far, the exact type of the defects has not yet been identified. Using computational methods such as density functional theory and transport simulations, we aim to make progress in determining their nature.

Type of Work
Theory & Simulation

Prerequisites
We are seeking a candidate with a strong interest in computational materials science. Basic programming skills (e.g. in Python or MATLAB) are required as well as a fundamental knowledge of solid-state physics. Prior experience with density functional theory or transport simulations is *not* required.



$4H-SiC/SiO_2$ structure with a defect

Status: Available
Looking for 1 semester project student

Interested candidates please contact: Colin Kälin (ckaelin@ethz.ch)
ETH Professor: Prof. Mathieu Luisier (mluisier@iis.ee.ethz.ch)