Ab initio calculations of spin defects

Available as B.Sc. or M.Sc. project or as special course

Background:

The section for atomic-scale materials design (CAMD) at DTU-Physics develops and applies *ab initio electronic structure calculations* to discover new materials for **quantum technology and green energy**. *Ab initio* calculations solve the quantum many-body problem of electrons in a solid, and thereby can predict physical properties of real materials with an accuracy comparable to experiments without any free parameters using the atom structure of the material as input.

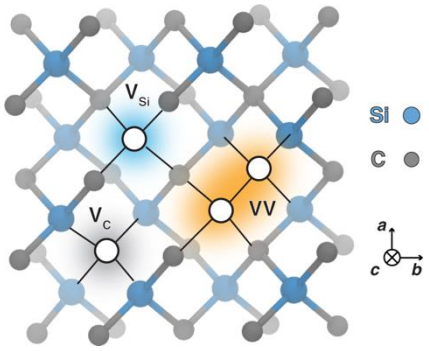
Ab initio calculations are used extensively both in academia and in the industry to model materials and molecules for various types of applications.

The CAMD section develops an in-house Python electronic structure code GPAW, which will be used in this project.

GPAW documentation: https://gpaw.readthedocs.io
GPAW review article: https://doi.org/10.1063/5.0182685

Project description:

You will use *ab initio* calculations to model spin defects realized as crystal point defects in a solid (similar to the NV center in diamond). Once familiar with the computational methodology you will explore novel types of spin defects and quantify their potential as a qubit system. The goal is to identify defects with spin ground state (doublet or triplet) that are optically accessible, good stability properties, and with long spin coherence times that can be read and initialized optically.



Different point defects in a SiC crystal. Figure adapted from *Nature Comm.* **12,** 6325 (2021)

Skills and knowledge acquired:

Atomic-scale materials simulations ; single-photon emitters ; running large-scale simulations on a supercomputer ; Python programming.

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GoogleScholar: https://scholar.google.dk/citations?user=NxOTQRcAAAAJ&hl=da