Exploring point defects as qubit candidates in cubic boron nitride

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1 Introduction

Quantum technology (QT) and quantum computing in general have opened a wide world of research in the solid state physics. This new field uses the fundamental principles of quantum mechanics such as superposition and entanglement, which are characteristics of qubits. A qubit is a basic unit of quantum computing that, unlike classical computing, can be initialized in a superposition of distinct states. In addition to quantum computing, qubits are the basic building block for quantum sensing and quantum communication as well. Currently, the physical platforms to implement qubits are in most cases based on superconducting materials, which operate at cryogenic temperatures (near to absolute zero). The low temperatures are necessary to make sure the qubits are stable with long lifetime or coherence time. This is to have enough time to perform operations and read-out the qubit state before the information is lost due to noise or decoherence.

To generate these conditions, where the qubit's lifetime is long (long coherence time), it is necessary to purchase costly equipment and use advanced quantum materials with specific properties (e.g., superconducting material platform). This is a challenge for building new computing technology, as we would want a technology that is scalable, sustainable and widely available.

For these reasons, it is very important to make advances in quantum technology towards a scalable and sustainable platform. That means, looking for new quantum materials that can replace superconducting materials. In addition, we are looking for new materials that can work as a qubit platform at room temperature.

A good option in terms of cost and the potential that has been shown in recent research is semiconducting materials. Semiconductors allow the creation and manipulation of qubits in several different ways. They also allow for the possibility of operation at room temperature.

A very interesting way to create qubits in semiconductors is through the point defects. Importantly, the material must meet certain criteria for quantum compatible point defects to be present [1]. The term point defect refers to intrinsic or extrinsic imperfections in the crystal like vacancies and impurities [2]. This new field has experienced rapid development in the scientific world, both theoretically and experimentally, since it is very promising and has the potential for scalable and room temperature quantum devices. Currently, a big trend in the field is the search for new semiconductor materials for the advancement of point defect based QT.

The most famous material platform for point defect based QT is diamond. However, diamond devices are challenging to fabricate and control. Therefore, there is an ongoing search for new materials to replace diamond in future quantum technologies [3]. Currently, semiconductors like Si and SiC are widely studied because of a wide variety of point defects that act as qubits and single photon emitters (SPEs). Cubic Boron nitride (c-BN) is also a material that is very interesting to study. c-BN is a semiconductor material that was predicted through machine learning methods as a suitable candidate for quantum technology [3]. In addition, c-BN has properties such as a wide band gap and low spin orbit coupling that are known to be useful for QT applications [1].

2 Project overview

c-BN, a semiconductor material with an ultra-wide band gap, will be the object of study in this thesis. The study of this novel material will be carried out by considering different point defects and their potential for QT applications. The selection of defect candidates to study in an initial screening process will be based on the available literature, and especially promising defects will be chosen to be studied in more detail.

The main idea of this thesis project is to identify defects in c-BN that can be used as qubits in a quantum platform. Simulations using Density functional theory (DFT) for point defects will be very important to obtain calculations that provide us with information about which defects are suitable for qubits. It will be important to carry out calculations of initial defect properties for several defects, including formation energy diagrams, spin state and zero-phonon line (ZPL) energy.

The project can be grouped into five main tasks:

1. DFT calculations of properties of bulk c-BN including band gap, lattice parameters, density of states, and band structure. Here we will also perform convergence tests and investigate the suitability of different exchange-correlation (XC) functionals (PBE, r2SCAN and HSE06).
2. Initial screening of multiple defect candidates based on available literature [4, 5]. Here we will calculate defect properties like defect stabilities, formation energy diagrams, ZPL energies, and spin states.
3. Exploration of novel methods for computing qubit properties of point defects.
4. Selection of a few defects (2 - 4) to look at in further detail. Here we will calculate defect properties like emission line shapes, spin coherence times, excited states, and time-dependent properties.
5. Experimental measurements using photoluminescence (PL) to explore defects in c-BN. The material will be grown by another master student in the LENS group.

Codes such as the Python cluster-correlation expansion (PyCCE) [6] and Without empty states (WEST) [7,,8] are novel tools to calculate qubit properties like spin coherence time and time dependent effects. Therefore, we aim to include them within this thesis project. Furthermore, WEST is a package that gives us the possibility of performing calculations such as quantum defect embedding and time-dependent DFT. The proposal to perform this last task will be taken into account depending on the relevance of the particular defect under study and the time available to carry it out, since it is a task with a high degree of complexity.

As the aim is to perform both theoretical and experimental research, some of the samples grown by another master's student in the laboratory will be used. This will be used to try to make and measure point defect qubit signals using photoluminescence.

3 Methodology

DFT is a ground-state computational technique that is invaluable to solid state physics. In the semiconductor physics field, it is very important since through modeling it allows us to extract important information from the material like band gap and density of states (DOS). But not only that, in the study of point defects we can also predict the stability of defects and transition levels using DFT calculations.

To perform these calculations, it is necessary use a platform (software) where we can simulate the material by applying DFT. Vienna Ab initio Simulation Package (VASP) [9,10] is a useful tool for these calculations, since it allows us to simulate materials to atomic scale.

In principle, using VASP we can calculate a solution to a many-bodies system (solve the Schrödinger equation) with pseudopotentials like local-density approximation (LDA), generalized gradient approximation (GGA), meta-GGA and hybrid functionals like the HSE06 functional.

PyCCE is a package to simulate the dynamics of a spin qubit interacting with a spin bath using the cluster-correlation expansion method. Mainly this code will be used to predict the spin coherence time of quantum defects.

Other types of code that could used are time-dependent DFT and quantum embedding, which are within the WEST package. This allows us to study models for excited-state and time-dependent effects of defects.

4 Progress plan

Scheduled semester	**Planned activity**
Fall 2023	Courses: - Modern quantum mechanics (FYS4110) - Quantum mechanics for many-particle systems (FYS4480) - Condensed matter physics II (FYS4430) - Follow Quantum mechanical modelling of nanomaterials (FYS-MENA4111) • Write project description • Read literature about DFT, quantum technology and c-BN • Start learning DFT calculations • Perform introductory DFT project on SiC in FYS-MENA4111 • Participate in Generic Competence seminars
Spring 2024	Courses: - Computational Physics II: Quantum Mechanical Systems (FYS4411) - Quantum computing and quantum machine learning (FYS5419) - Material Science of Semiconductors (FYS4310) • Build initial DFT model of c-BN * Perform convergence test for unit cell and supercell * Compare different exchange-correlation functionals (PBE, r2SCAN and HSE06) * Calculate bulk properties of c-BN (band gap, lattice parameters, density of states, band structure, phonons, dielectric constant) • Participate in Generic Competence seminars ⧫ Milestone: Choose initial relevant defects in c-BN for QT based on literature
Fall 2024	• Perform DFT calculations for defect properties of initial defect selection * Formation energy diagrams and defect stability * Spin state and symmetry analysis * Electronic structure and localization factors * ZPL emission energies • Read documentation and perform test of Py-CCE code • Read documentation and perform test of WEST code • Photoluminescence measurements to look for quantum emitters in c-BN grown by sputtering by another master student at LENS • Participate in Generic Competence seminars • Start writing master's thesis ⧫ Milestone: Choose 1-2 defects to perform calculations of quantum properties

Spring 2025	• Calculate quantum properties for 1-2 promising defects:
	  * Phonons and emission line shape
	  * Excited state lifetime
	  * Zero-field splitting
	  * Spin coherence time
	• Data analysis
	• Finalize calculations
	• Write master thesis
	• Thesis defense

5 Risk assessment

The project will involve some characterization of semiconductor materials. The groups and research infrastructures (MiNaLab) involved have internal procedures for risk evaluations related to laboratory work and materials. Relevant risk evaluations have already been conducted for many of the potential materials regarding the general aspects of the materials that will be investigated. Risk evaluations of new materials and procedures that are introduced by the project will be conducted in accordance with the internal procedures in the MiNaLab.

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