Atomically Thin Layers For Energy Harvesting And Storage - Project Planning Document.

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1. Year 1 - Experimenting with materials and simulation.

1.1. Project Administrative work

1.1.1. COSHH and Risk Assessments: The initial stage of the project was to process relevant health and safety assessments of relevant chemicals and lab equipment. This was done by attending various lab inductions and discussing the project with lab technicians. Training on equipment, such as the scanning electron microscope and nanoparticle printing, will be done when they are required for the project.

1.1.2. Project Planning and Approval: The first draft for this was completed and reviewed before submission.

1.1.3. CDT Training: The CDT Training was split into various modules:

- C1: This module is an introduction to the CDT which is carried out at Kielder Observatory, where the students are given talks about astronomy, astrogeology, meteorology and more.
- C2: This module is covered over two weeks. Week 1 covers topics including solar cells (mechanisms, characterisation and fabrication techniques), electrochemistry, battery technologies, photochemistry and photo-catalysis, thermal energy storage, wind turbines (power, materials and corrosion). Week 2 covers topics including studies on atomistic simulation, H_2 fuel cells, application of catalysis, new materials in Li and Na-ion batteries, polyoxometalates chemistry, nanomaterials and nanochemistry, aerodynamics of wind energy, solid state NMR, generator and grid connection of wind, XPS, XRD, Raman and Scanned Probe Microscopy.

- CDT Week: Throughout this week, students present a brief introduction to their projects to industry partners, discuss their project in further detail at a scientific poster session, are inducted to equality diversity and inclusion, and visit the ORE Catapult site.
- C3: Responsible Research and innovation training on week 1 shows students how to self assess their projects to ensure they make responsible decisions throughout their project. In week 2, taught modules include data analysis, programming and publishing.

1.2. Experimental Work

1.2.1. ZnO nanowire fabrication process: Through chemical bath deposition, ZnO nanowires will be grown from a ZnO seed layer. This will be analysed with the electron microscope and EDS to capture the morphology and composition of the nanostructure. Room temperature PL with a 375nm laser, as well as isothermal gas adsorption analysis will be used to characterise the surface before and after hydrogen adsorption. UV-Vis will be used to test if the nanowire length can be measured.

1.2.2. ZnO confinement: ZnO nanowires will be grown on a ZnMgO thin film using CBD. A ZnMgO cap layer will be deposited by either sputtering or ALD to confine the ZnO material. This will be tested for conduction across the ZnO. This will then be described in terms of thickness and conductivity as a function of Mg concentration to establish ideal fabrication conditions.

1.2.3. Milestone 1: At this point in the project, fabrication experiments should be completed for hydrogen adsorption onto bare ZnO nanowires, as well as measures taken to create ZnO confinement for sensing.

1.2.4. ZnMgO/ZnO/ZnMgO sensor Using the nanoparticle printer, Ag nanoparticles will be deposited on the surface of the device, allowing for full functionality of the gas sensor. This will be tested using similar gas adsorption methods as before, measuring the current in the charged and uncharged state.

1.2.5. Nanowire orientation: Using ALD, ZnMgO seed layer will be deposited on bare glass to compare the orientation of the ZnO nanowires with the sputtered ZnMgO seed layer. The ALD seeded nanowires will then be integrated to a sensor and compared to the previous sensor. This will give insight to the effects of orientation on gas adsorption and sensing.

1.2.6. Milestone 2: At this point in the project, two sensors with differing nanostructured ZnO morphologies will be fabricated and modified with ALD or sputtered ZnMgO layer to enable gas sensing.

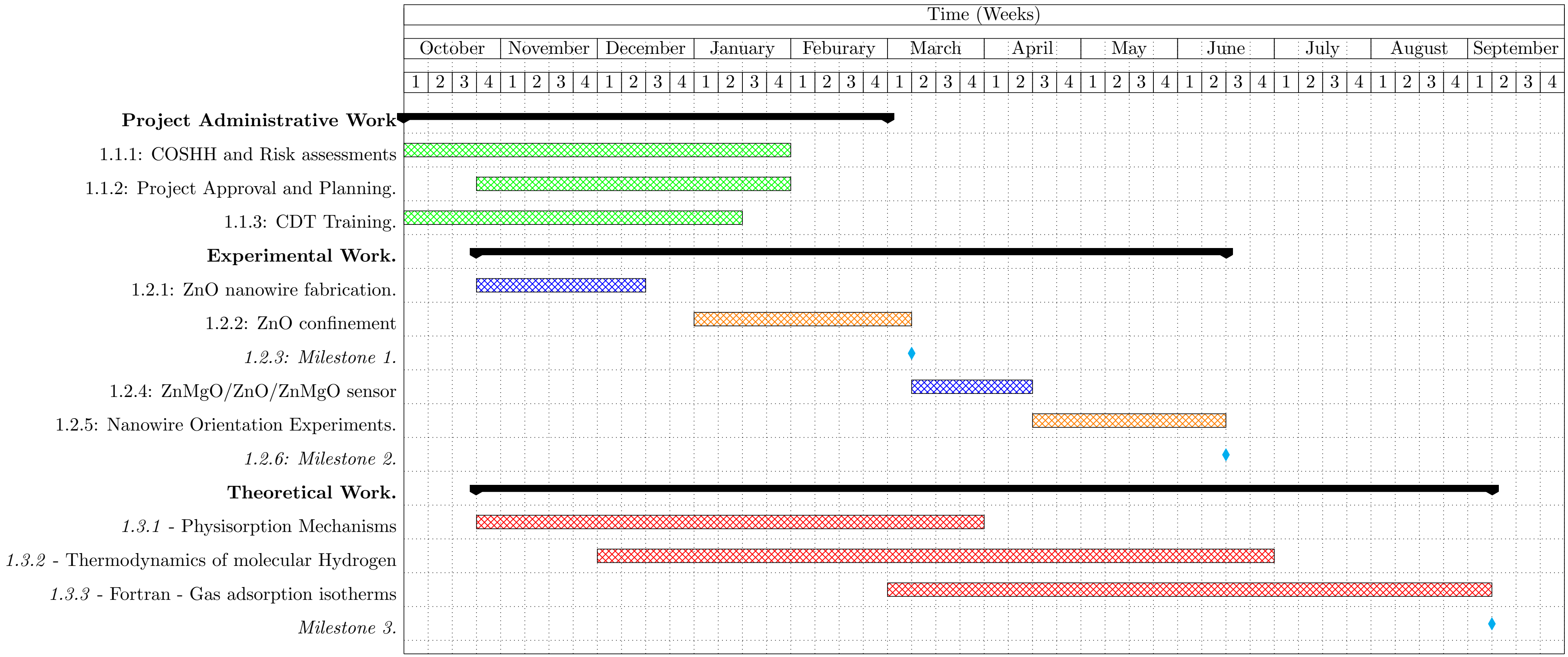
1.3. Theoretical work

1.3.1. Physisorption mechanisms: As a foundation for the molecular simulation model, the physical adsorption of gas using a 3D quantum mechanical oscillator within a Lennard-Jones potential will be studied. This will consider the perturbation of diatomic hydrogen, firstly by looking at Coulombic energy contributions for the system, working towards a description of the van der Waals forces along a ZnO nanowire.

1.3.2. Thermodynamics of molecular hydrogen: To describe the adsorption accurately, the kinetics of the gas must first be studied, to determine the probability of the gas being adsorbed. This will be done using a statistical mechanics approach.

1.3.3. Fortran code for molecular dynamics modelling: To compute adsorption isotherms, Fortran programming will be used with the General Utility Lattice Program. Initially, monatomic gasses will be modelled to adsorb onto metallic surfaces, before exploring diatomic molecules in pores and on nanowires.

1.3.4. Milestone 3: At this stage of the project, all data analysis and calculations should be concluded into an end of year report.



One year Gantt Chart showing the project management stages in green, experiments in blue, analysis/characterisation in orange and theoretical work in red. The milestones are represented as cyan diamonds.

2. Four Year Plan

Throughout this PhD, this project will investigate the utility of nanostructures and atomically thin layers of metal oxides for energy conversion and storage. This will include one novel energy storage method and one popular storage method, and energy generation in solar cells.

For year one, this project will be focused mainly around the implementation of ZnO nanostructures for room temperature hydrogen densification, for the purpose of investigating storage and sensing applications.

During second year, the main focus will be around implementing the computational solutions into designing experiments for fabricating optimised nanostructures for hydrogen storage. This will be followed with some research on using alternative nanostructures, such as nanoparticles or nanospheres for hydrogen storage.

During third year, the project focus will be on novel ways of using nanostructures and atomically thin layers for photovoltaic applications, such as lensing and electron confinement.

In the final year, prior to the thesis writeup, the research focus will be on implementing nanostructures and metal oxides with dielectrics in capacitors.

2.1. Year 1

- Fabricate and Characterize ZnO nanowires using CBD method.
- Grow ZnO nanowires from ZnMgO seed and deposit ZnMgO on surface using ALD and measure volumetric H_2 adsorption.
- Create a H_2 gas sensor using the previous heterostructure using ALD and nanoparticle printer.
- Use sputtering and ALD to vary seed layer roughness and compare storage between various nanowire orientations.

2.2. Year 2

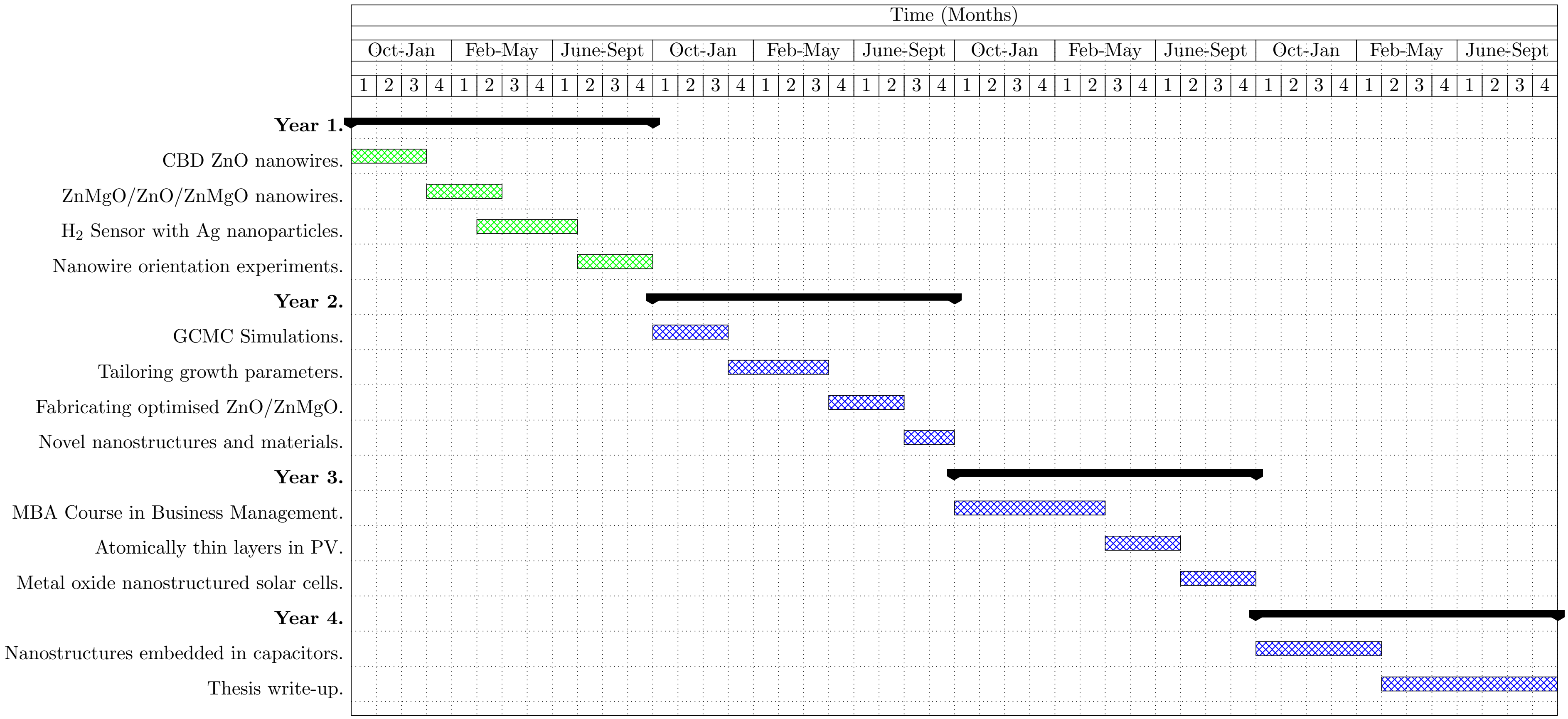
- Grand Canonical Monte Carlo simulations based on Hydrogen adsorption data.
- Tailoring experimental growth parameters for ZnO nanowires and fabricating sensors based on the new parameters.
- Alternative nanostructures and materials using ALD.

2.3. Year 3

- MBA - Business Management.
- Atomically thin layers in photovoltaics.
- Metal oxide nanostructured solar cells.

2.4. Year 4

- Nanostructures embedded in capacitors.
- Thesis write-up - Metal oxides and nanostructures using atomically thin layers for energy harvesting and storage.



4 year gantt chart showing current year ongoing project in green, future research in blue. Years are indicated as black bars.