

Summer Research Project (Undergraduate Placement)

Title

## Modelling irradiation of wide band gap semiconductor $\text{Ga}_2\text{O}_3$

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Type of Project: Computational/Theoretical

### Project Overview

Wide band gap semiconductors are required for power electronics, as standard silicon-based components are less robust and face serious challenges.  $\text{Ga}_2\text{O}_3$  is an ideal candidate for applications, with its 4.9 eV band gap and a nominal critical field strength of 8 MV/cm. The supervisor and his collaborators have been studying  $\text{Ga}_2\text{O}_3$  and its alloys over the past few years. Among the potential applications of  $\text{Ga}_2\text{O}_3$ , there is space electronics. Electronic devices on satellites must operate under constant irradiation of charged particles. Predicting device behaviour and failure in these conditions is not trivial. In this project, we consider a simple model of proton irradiation of  $\text{Ga}_2\text{O}_3$ .

### Project Description

The successful candidate will model  $\text{Ga}_2\text{O}_3$  in the so-called warm-dense matter regime, using existing electronic structure codes such as VASP or OCTOPUS. The expected results will help clarify the mechanical and phase behaviour of  $\text{Ga}_2\text{O}_3$  in a relative unexplored regime. All calculations will be run on the Northern Ireland High Performance Computing (NI-HPC) facilities.

### Background and Skills

The project is suitable for advanced undergraduate students in physics, applied mathematics, or related fields.

Required: Basic programming skills and an interest in either plasma or condensed matter physics.

Not required: Prior experience with electronic structure calculations or high-performance computing.

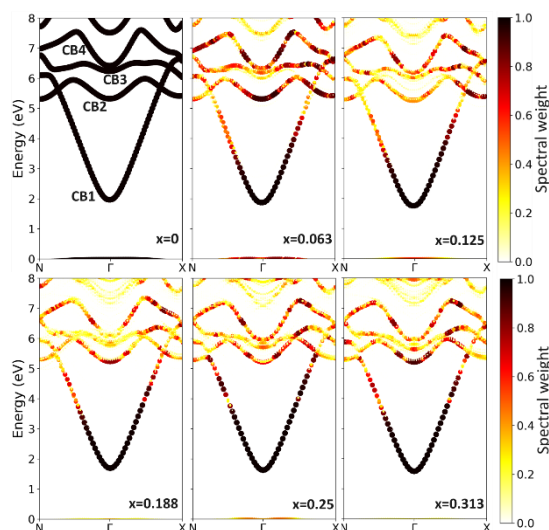


Figure 1: Band structures of  $\text{Ga}_2\text{O}_3$  alloys (from Ref. 2).

### Useful references

1. S. J. Pearton, F. Ren, M. Tadjer and Jihyun Kim; *Journal of Applied Physics*, **124**, 220901 (2018)
2. M.A. Fadla, M. Grüning and L. Stella, *ACS omega*, **9**, 15320 (2024).
3. M.A. Fadla, M. Grüning and L. Stella, *Phys. Rev. Materials* **9**, 105002 (2025).