Project Title: Radiation damage in the wide band gap semiconductor Ga_2O_3

Supervisor(s): Dr Lorenzo Stella

Email contact: l.stella@qub.ac.uk

Type of Project: COMPUTATIONAL/THEORETICAL

Helpful existing knowledge: A previous knowledge of quantum mechanics is required. A previous experience with computational methods is desirable, but not necessary.

Funding status: Awaiting funding

Project Description

Wide band gap semiconductors are required for power electronics, as silicon-based components are less robust and face serious challenges. Ga_2O_3 is an ideal candidate for applications, with it 4.9 eV band gap and a nominal critical field strength of 8 MV/cm. However, predicting the device failure condition is not trivial, as the microscopic description of dielectric breaking is complex, involving different mechanisms and timescales. In this project, we aim at modelling the dielectric breaking of Ga_2O_3 using first principles atomistic modelling and macroscopic approaches based on finite element/volume methods.

The results of this project can inform material and device modelling for power application such as energy generation from renewable sources (solar, wind, hydroelectric) and power converter for hybrid vehicles.

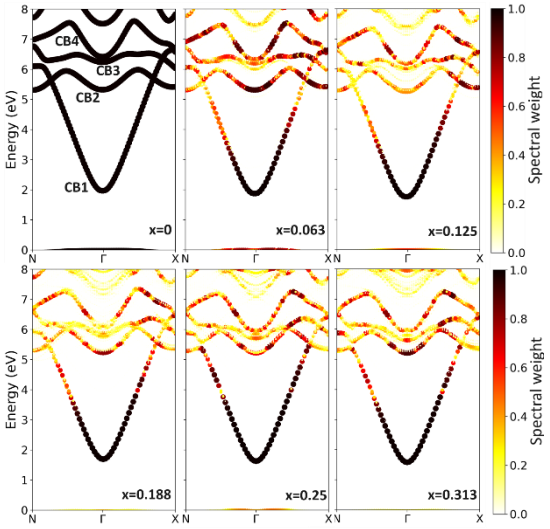

Figure 1: Band structures of Ga2O3 alloys (see ref. 2)

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).