Contribution ID: **288** Type: **Poster Presentation**

First Principles Study of Nitrogen Dopant-Vacancy Complexes in Graphane

We use first principles calculations to characterize four types of dopant-vacancy point defects in the two dimensional material graphane for the purpose of quantum computing. The point defects we consider in this contribution are NcHv, NcCHv, NchHv, NchCHv and their various charge states. We derived the formation energies and other electronic properties of these point defects. Analysis of the defect level diagrams shows that NcHv is a deep point defect that can be potentially utilised as a qubit like the prototype NV centre in diamond.

Apply to be considered for a student ; award (Yes / No)?

Yes

Level for award;(Hons, MSc, PhD, N/A)?

PhD

Primary authors: Mr MAPINGIRE , Hezekia (University of Pretoria); Dr MAPASHA , R. E (University of Pretoria)

Presenter: Mr MAPINGIRE , Hezekia (University of Pretoria)

Session Classification: Poster Session

Track Classification: Track G - Theoretical and Computational Physics