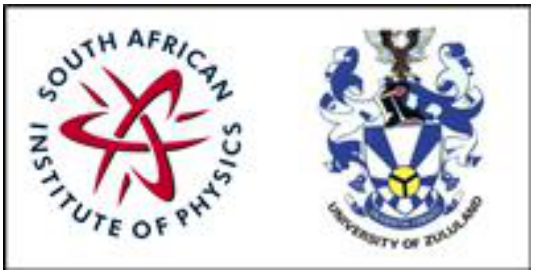

Contribution ID: **509** Type: **Oral Presentation**

Nitrogen-Vacancy colour centre in diamond characterization using QUANTUM ESPRESSO

Wednesday, 10 July 2013 16:00 (20 minutes)

Abstract content
   (Max 300 words)

The model of electronic structure and calculations using Quantum Espresso is presented. Defects in diamond, the nitrogen-vacancy in particular, is a promising candidate for realizing qubits for a number of applications such as quantum computing, high spatial resolution imaging, quantum information processing, magnetic field sensing, single photon emission and biocompatibility. Diamond defects can be identified by means of density functional theory (DFT) electronic calculations using traditional local functionals. Time-dependent DFT (TD-DFT) is used to calculate the electron – hole interactions of the system of the NV centre. This allows the study of the energetic stability and electronic structure of the negatively charged NV centre. The charge and spin distribution of the centre in diamond for both ground and excited states are analysed by the use of ab initio supercell calculations.

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

Yes

Level for award
 (Hons, MSc,
   PhD)?

PhD

Main supervisor (name and email)
and his / her institution

Professor Petruccione, petruccione@ukzn.ac.za, University of KwaZulu-Natal

Would you like to
 submit a short paper
 for the Conference
 Proceedings (Yes / No)?

Yes

Primary author: Mr ZULU, Bheki (University of KwaZulu-Natal)

Co-author: Prof. PETRUCCIONE, Francesco (University of KwaZulu-Natal)

Presenter: Mr ZULU, Bheki (University of KwaZulu-Natal)

Session Classification: Theoretical

Track Classification: Track G - Theoretical and Computational Physics