Contribution ID: **381** Type: **Oral Presentation**

Theoretical characterization of beryllium and nitrogen co-doped graphene: a proposed p-type semiconductor for nanoelectronic devices

Wednesday, 5 July 2017 11:30 (20 minutes)

Ab-initio calculations within the framework of density functional have been performed to study the electronic properties of Be and N co-doped graphene. The results have been compared with that of Be-doped, N-doped and pristine graphene. The effect of doping and isomerization on the electronic properties of these systems have been studied by varying the impurity concentrations of Be-doped and N-doped graphene systems from 3.13 through 12.5 %, while for Be and N co-doped graphene, the concentration have been varied from 6.25 through 25.0 % impurity concentration.The formation energies of the systems with different impurity configurations were calculated to examine their relative stabilities. It was found that for Be-N co-doped graphene, N and Be coexisting as the nearest neighbours is energetically the most favourable configuration. Moreover, at the same impurities concentration, Be-N co-doped graphene was observed to be more stable than Be-doped graphene due to its lower formation energy. Thus these results reveal that it is much easier to synthesize Be-N co-doped graphene than to synthesize Be-doped graphene. Hence, the relatively high formation energy of Be-doped graphene could be the reason why the system is yet to be synthesis experimentally.
The results of the electronic structure calculations reveal that Be-N co-doped and Be-doped graphene are p-type semiconductors while N-doped graphene has been verified to be n-type semiconductor.
For all the doped systems considered, it was observed that the size of the band gap increases with impurity concentration with respect to the aforementioned energetically most favourable isomer. At impurity concentration of 3.13 %, a minimum band gap of 0.44 eV and 0.21 eV was realised for Be-doped and N-doped graphene respectively while at 12.5 % corresponding maximum gap of 1.41 eV and 0.6 eV were observed. Besides, Be-N co-doped graphene were found to have a minimum band gap of 0.43 eV at 6.25 percent and a maximum gap of 1.54 eV at 25.0 % impurity concentration.
The results of our study demonstrate that the band gap of graphene can be tailored to meet the requirements of specific applications in nanoelectronic devices.

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

Yes

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

PhD

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

Prof. Ncholu Manyala
ncholu.manyala@up.ac.za
University of Pretoria

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

No

Primary author: Mr OLANIYAN, Okikiola (UP)

Co-authors: Mr KHALEED, Abubakar (University of Pretoria); Dr MAPASHA, Edwin (University of Pretoria); Mr IGUMBOR, Emmanuel (University of Pretoria); Dr MANYALA, Ncholu (University of Pretoria)

Presenter: Mr OLANIYAN, Okikiola (UP)

Session Classification: Theoretical and Computational Physics 1

Track Classification: Track G - Theoretical and Computational Physics