Contribution ID: **31** Type: **Poster Presentation**

Computational simulations of graphene and carbon nanotubes

Thursday, 12 July 2012 17:30 (2 hours)

Abstract content
   (Max 300 words)

Molecular dynamics simulations are used to study the relative stability of graphene and carbon nanotubes. The formulation of the Tersoff bond-order potential was used to investigate the energetic stabilities and thermodynamics properties through a range of temperature. The structural properties were studied using the radial distribution effects functions. The thermodynamics effects were studied using the energy-temperature plots. Similarities and differences in graphene and carbon nanotubes are discussed.

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

YES

Level for award
 (Hons, MSc,
   PhD)?

MSC

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

Dr TE MOSUANG(thuto.mosuang@ul.ac.za) UNIVERSITY OF LIMPOPO

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

NO

Primary authors: Ms SHAI, MOSHIBUDI (university of limpopo); Dr MOSUANG, THUTO (UNIVERSITY OF LIMPOPO)

Co-author: Prof. RAMMUTLA, ERASMUS (UNIVERSITY OF LIMPOPO)

Presenter: Ms SHAI, MOSHIBUDI (university of limpopo)

Session Classification: Poster Session

Track Classification: Track G - Theoretical and Computational Physics