Contribution ID: **379** Type: **Poster Presentation**

Molecular dynamics studies of some carbon nanotubes chiral structures

Tuesday, 8 July 2014 17:10 (1h 50m)

Abstract content
   (Max 300 words)
Formatting &
Special chars

Structural and equilibrium properties of armchair (cnt(12,12)) and two chiral (cnt(10,12) and cnt(12.10) carbon nanotubes are studied using classical molecular dynamics. The formulation uses the Tersoff potential under the NVT ensemble to study these properties. Structural properties are studied using the radial distribution and structure factor functions. The equilibrium properties are studied using the total energy against lattice parameter variation. Similarities and differences in cnt(12,12), cnt(10,12), and cnt(12,10) symmetries are discussed.

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

No

Level for award
 (Hons, MSc,
   PhD)?

none

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

Yes

Primary author: Dr MOSUANG, Thuto (University of Limpopo)

Co-authors: Prof. RAMMUTLA, Erasmus (Univerisity of Limpopo); Ms SHAI, Moshibudi (University of Limpopo)

Presenter: Dr MOSUANG, Thuto (University of Limpopo)

Session Classification: Poster1

Track Classification: Track G - Theoretical and Computational Physics