Contribution ID: **492** Type: **Poster Presentation**

Computational study of O vacancy and Ti doped tin-dioxide(SnO₂)

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Abstract content
   (Max 300 words)

The Classical molecular dynamics simulations focused on the structure,stability and possible phase transformation in anatase to rutile tin dioxide (SnO₂) is being investigated. This is done relative to titanium and oxygen vacancy defects in tin dioxide.The radial distribution functions suggest a possible structural mechanism for the transformation. Thermodynamic properties obtained from energy-temperature graphs are being discussed in relation to experiments. Equilibrium properties of rutile and anatase phases also suggest the stable phase.

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: Mr NTIMANE, NDUMA (UNIVERSITY OF LIMPOPO); Dr MOSUANG, THUTO (UNIVERSITY OF LIMPOPO)

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

Presenter: Mr NTIMANE, NDUMA (UNIVERSITY OF LIMPOPO)

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