Contribution ID: **399** Type: **Poster Presentation**

# Structural properties of some defects in tin-dioxide (SnO<sub>2</sub>)

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

## Abstract content <br>   (Max 300 words)

The stability of some point defects in tin-dioxide is being examined. Particularly, an oxygen vacancy and Titanium impurity in tin-dioxide are being modelled to understand whether they can enhance or impede tin-dioxide properties. Classical molecular dynamics simulations focused on the structure and equilibrium properties of these defects is being used. The defect formation energies for the two defects type are used to determine the most stable defect. Calculations also give evidence of the possible mechanism for the anatase to rutile tin-dioxide phase transformation.

## Apply to be<br> consider for a student <br>   award (Yes / No)?

No

## Level for award<br> (Hons, MSc, <br>   PhD)?

N/A

## Main supervisor (name and email)<br>and his / her institution

TE Mosuang - thuto.mosuang@ul.ac.za
University of Limpopo

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

Yes

**Primary authors:** Mr NTIMANE, James (University of Limpopo); Dr MOSUANG, Thuto (University of Limpopo)

**Co-author:** Prof. RAMMUTLA, Erasmus (University)

**Presenter:** Mr NTIMANE, James (University of Limpopo)

**Session Classification:** Poster Session

**Track Classification:** Track A - Division for Condensed Matter Physics and Materials