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# Molecular dynamics studies of Schottky and Frenkel defects in cerium dioxide

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## Abstract content <br>   (Max 300 words)<br><a href="http://events.saip.org.za/getFile.py/a target="_blank">Formatting &<br>Special chars</a>

Schottky and Frenkel defect energies in cerium dioxide are studied using the classical molecular dynamics. Buckingham potentials are used to understand the cerium-oxygen and oxygen-oxygen interactions in the bulk and defect structures. The formulation uses the NVT Evans ensemble to obtain the various defect energies. Oxygen and cerium vacancy defect energies relative to bulk cerium dioxide total energies are used to get more insight on cerium dioxide as a catalyst in exhaust systems. Oxygen ions transport properties are studied using the time-dependent mean square displacement. The anion Frenkel-pair defect is the most favourable form of intrinsic ionic defect.

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

No

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

Hons

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

Thuto Mosuang, thuto.mosuang@ul.ac.za, University of Limpopo

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Yes

**Primary authors:** Prof. RAMMUTLA, Erasmus (University of Limpopo); Ms LEKOKO, Oldoria (University of Limpopo); Dr MOSUANG, Thuto (University of Limpopo)

**Presenter:** Dr MOSUANG, Thuto (University of Limpopo)

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