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# Structural and Dynamical Properties of Pentlandite Nanostructures: Atomistic Simulation Approach.

*Thursday, 11 July 2019 15:00 (2 hours)*

Atomistic simulations were carried out to study the melting behaviour of pentlandite nanostructures, in order to understand their structural and dynamical properties. Pentlandite is a major precious metals-bearing mineral and plays a very important role in mining. Precious metal ores co-exists with base metals either as solid-solution and intergrowths, hence rendering its detailed understanding important for efficient extraction of these precious metals. This work relates to problems in applied areas such as mineralogy, geophysics and geochemistry, whereby phase transition is modified by impurities, so there is the additional concern of the effect of temperature. Computational modelling technique, molecular dynamics (MD) was performed to provide atomic or molecular level insights of the structural and dynamics of pentlandite nanostructures. The effect of temperature on different sizes of nanostructures was determined via the structural and dynamical properties; namely radial distribution functions (RDFs), variation of energy as a function of temperature and diffusion coefficients. Both mechanisms reveal that as a size of nanostructure increases, the melting temperature increases.

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

No

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

N/A

**Primary author:** Dr MEHLAPE, Mofuti (University Of Limpopo)

**Co-author:** Prof. NGOEPE, Phuti (University of Limpopo)

**Presenter:** Dr MEHLAPE, Mofuti (University Of Limpopo)

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