Contribution ID: **215** Type: **Poster Presentation**

Computational Studies of Pentlandite Mineral: Structural and Dynamical Properties Probed by Molecular Dynamics

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. In order to extract the precious metals from the ores effectively it is necessary to study and understand structural and physical properties, of pentlanidte mineral in detail. 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) is applied to investigate structural and physical properties of nickel rich pentlandite (Fe4Ni5S8). Radial distribution functions (RDFs) and mean square displacement (MSD) are used to establish the effect of temperature on the pentlandite mineral. The MD results are found to compare well with the experimental results.

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

No

Level for award;(Hons, MSc, PhD, N/A)?

N/A

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Session Classification: Physics of Condensed Matter and Materials

Track Classification: Track A - Physics of Condensed Matter and Materials