National Conference on Recent Advances in Science, Engineering, Humanities, and Management (NCRASETHM - 2024)
28th January, 2024, Banquet, Noida, India.

CERTIFICATE NO : NCRASETHM /2024/C0124140

COMPUTATIONAL INVESTIGATION OF THERMO-PHYSICAL PROPERTIES IN COPPER METALLIC NANOPARTICLES

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ABSTRACT

Computational investigation of the thermo-physical properties of copper metallic nanoparticles plays a pivotal role in understanding and predicting their behavior at the nanoscale. This approach employs advanced computational techniques, such as molecular dynamics (MD) simulations, density functional theory (DFT), and finite element analysis (FEA), to explore the unique properties that emerge when copper is reduced to nanoparticle form. These properties, including thermal conductivity, melting point, heat capacity, and electrical conductivity, differ significantly from bulk copper due to the influence of quantum and surface effects. Computational methods help in systematically analyzing how variables like particle size, shape, surface morphology, and the surrounding environment impact these properties. For instance, MD simulations can reveal how the rapid diffusion of atoms on the surface of copper nanoparticles affects thermal conductivity, while DFT calculations can provide insights into electronic structure changes. This in-depth understanding is essential for optimizing the performance of copper nanoparticles in practical applications, such as improving heat dissipation in microelectronics, enhancing catalytic processes, and developing advanced medical imaging techniques. Furthermore, computational investigations enable the exploration of how surface modifications or coatings could mitigate issues like oxidation and agglomeration, enhancing the stability and efficiency of copper nanoparticles in real-world applications.