National Institute of Technology Rourkela

Registration Seminar

Seminar Title	: Interatomic Potential Development for Metallic Systems
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Venue	: Seminar Room: MM Annex Building
Date and Time	: 25 Jun 2024 (10:30 AM)
Abstract	: Molecular Dynamics (MD) simulation helps to investigate different aspects of an alloy system, starting from scratch. In this regard, interatomic potential is important in starting the simulation procedure. We are conducting our research to develop interatomic potentials, particularly Embedded-Atom Method (EAM) potentials, and implementing these potentials in MD simulations to investigate several aspects of different metallic systems. The force-matching approach has been taken to develop the EAM potentials first. Then, the optimization to converged Density-Functional Theory (DFT) data sets has been carried out to make reliable and appropriate potentials for different metallic systems, for example, Palladium-Barium and Rhodium-Barium alloy systems. Properties like density, elastic constants, bulk modulus, Poisson&rsquos ratio, and thermal conductivity have been calculated through MD simulations using those developed EAM potentials and validated these properties with DFT-based results to examine the accuracy and performance of those potentials. Discrepancies in some places have been observed because of the difficulty fitting procedures. These developed EAM potentials have been used to calculate the melting points of the abovementioned alloy systems at different compositions.