

Physics Colloquium

Michigan Technological University

November 18 (Thursday) 4:00 to 5:00 pm
Room 139, Fisher Hall

Melting in finite sized systems

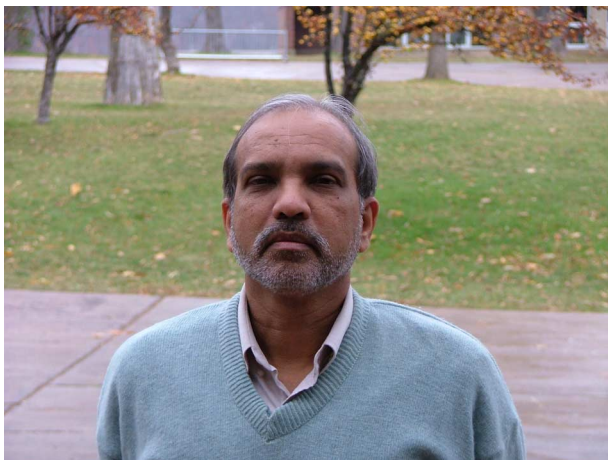
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Abstract

Finite temperature properties of clusters in the size range 10-400 atoms show rather intriguing behavior. Contrary to "common sense understanding", the melting temperatures in some clusters were observed to be higher than the bulk melting temperature. Specifically, Clusters of Tin and Gallium were found (experimentally) to melt at higher than bulk temperature at least by a few hundred K. A series of experiments on sodium clusters in the range of $N=55$ -300 were found to have rather irregular behavior in the Melting temperature. The peaks did not correlate to either geometric or electronic magic numbers. The talk will introduce the topic and examine some of the issues. The results obtained by using state of the art *ab initio* density functional molecular dynamics will be presented to explain observed "higher than bulk melting" in Gallium and Tin. The most recent work on sodium clusters (Na_{55} , Na_{92} and Na_{142}) which shows excellent agreement with the experimentally measured heat capacities will also be presented.

Biography



Dr. Dillip G. Kanhere is a Professor in the Department of Physics at the University of Pune, India (since 1992), and director of the Center for Modeling and Simulations at the University of Pune. Currently, he is a visiting Professor at MTU. Prof. Kanhere received his Ph.D. in Solid State Theory (in 1976) from the Indian Institute of Technology (IIT) at Kanpur. He is a fellow of Indian Academy of Science, senior associate of the International Center for Theoretical Physics (ICTP) Trieste, Italy and recipient of the prestigious Meghnath Saha award in theoretical science. His current research interests are physics of clusters,

strongly correlated systems, and density functional theory and its applications.