Phase transitions - A look from the atomic vibration perspective

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ABSTRACT

Phase transitions are ubiquitous in materials. For example, iron undergoes structural phase transitions from bcc-a to fcc-g phase at 1185 K and fcc-g to bcc-d phase at 1670 K before melting around 1811 K, and ferromagnetic phase transition below Curie temperature of 1043 K. In this talk, I will describe the structural, magnetic, and electronic phase transitions as seen from the atomic vibrations (aka phonons) perspective, and how these vibrations coupled with electrons and electron spins control a subtle competition of energetic and entropic free-energy components to govern the thermodynamics.

I will present results from three of our recent combined experimental (neutron and x-ray scattering) and theoretical studies. In particular, I will discuss the phonon-phonon coupling and improper ferroelectric phase transition in archetypal YMnO$_3$ [1], breakdown of phonons across the superionic phase transition in CuCrSe$_2$ [2], and a concomitant structural, magnetic, and electronic phase transition enabled by magnetically triggered phonon instability in h-FeS [3].


ABOUT THE SPEAKER

Prof. Dipanshu Bansal joined as an assistant professor in the Department of Mechanical Engineering at IIT Bombay in 2018. His research is focused on lattice dynamics and phase transitions of energy materials (see https://sites.google.com/view/spectroscopy-iitb/ for current research). Prior to the current position, Prof. Bansal was a postdoctoral researcher in the Mechanical Engineering and Materials Science department at Duke University (2017-18) and Oak Ridge National Laboratory (2015-17). His postdoctoral research focused on the study of "Quasiparticle coupling in the transport of heat, charge, and spin" using experimental neutron and x-ray scattering combined with first-principles electronic, lattice, and spin dynamics simulations. Prof. Bansal obtained his bachelor’s degree from IIT Kanpur in 2010, M.S., and Ph.D. from SUNY at Buffalo in 2012 and 2015, respectively. His Ph.D. work involved the study of anharmonic behavior in thermoelectrics, superconductors, and negative thermal expansion materials.

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