ME Seminar

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].

[1] Dipanshu Bansal, Jennifer L Niedziela, Ryan Sinclair, V Ovidiu Garlea, Douglas L Abernathy, Songxue Chi, Yang Ren, Haidong Zhou, and Olivier Delaire. Momentum-resolved observations of the phonon instability driving geometric improper ferroelectricity in yttrium manganite. *Nature communications*, 9(1):1–9, 2018.

[2] Jennifer L Niedziela*, Dipanshu Bansal*, Andrew F May, Jingxuan Ding, Tyson Lanigan-Atkins, Georg Ehlers, Douglas L Abernathy, Ayman Said, and Olivier Delaire. Selective breakdown of phonon quasiparticles across superionic transition in cucrse 2. *Nature Physics*, 15(1):73–78, 2019.

[3] Dipanshu Bansal, Jennifer L Niedziela, Stuart Calder, Tyson Lanigan-Atkins, Ryan Rawl, Ayman H Said, Douglas L Abernathy, Alexander I Kolesnikov, Haidong Zhou, and Olivier Delaire. Magnetically driven phonon instability enables the metal–insulator transition in h-fes. *Nature Physics*, pages 1–7, 2020.

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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