ACCMS-Global Research Center, SRMIST, Chennai India

Webinar #2

Prof. Umesh V. Waghmare

Theoretical Sciences Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, India

Title: Multi-Scale Modelling and Theory of Structural Phase Transitions

28th September 2021, 10.00 – 11.30 am IST

About speaker

Prof. Umesh V. Waghmare graduated with an Institute Silver Medal and a B.Tech in Engineering Physics (1990) from IIT-Bombay. He received a Ph.D. in Applied Physics from Yale University, New Haven in 1996 and carried out postdoctoral research at Harvard University (1996-2000). He joined JNCASR as Assistant Professor in 2000. He had been an Adjunct Professor in Birck Nanotechnology Center of Purdue University (2010-2012) and TIFR, Mumbai (2014-2017). He is currently a Professor in the Theoretical Sciences Unit, JNCASR (2009-present). His research group is working on development of Formalism and Methods, materials for Energy and Environment, multiferroics and dilute magnetic semiconductors, and mechanical deformation of materials. He has received numerous awards like Shanti Swarup Bhatnagar Prize for Science and Technology in 2010, Infosys Prize in Engineering and Computer Science in 2015, GD Birla award for scientific research in 2016, Distinguished Alumnus Award, IIT Bombay in 2017. He has published nearly five hundred papers with more than 31500 citations with a h-index 68. He has authored several chapters on various topics in 10 books. He has contributed several Outreach Programmes within India and Africa for promoting computational materials science. He has been a technical consultant to companies like General Electric, Tata Research, Design and Development Centre (TRDDC), Boeing, Shell and so on. He is Associate Editor of Nanoscale, and Editor of Pramana – Journal of Physics. He is a Member in National Academy of Sciences, Advanced Materials and Powder Research Institute (CSIR), Nano Science Advisory Group, Nano Mission, Government of India (2012-present). He is the Co-Founder of Breathe Applied Sciences Pvt Ltd, a start-up company for CO_2 reduction from 2016. URL: https://www.jncasr.ac.in/faculty/waghmare

Abstract*

Properties of a material are fundamentally determined by its structure, and hence sharp changes in its structure marking a structural phase transition have remarkable impact on its behavior. Symmetry breaking at such a phase transition typically is a cause for emergence of technologically important functional properties. For example, use of a ferroelectric in sensors, speakers or in memories is possible due to piezoelectricity and switchable dipole moments it exhibits as a consequence of broken inversion symmetry. For development of advanced functional materials, it is thus highly desirable to have material-specific theory of structural phase transitions, which often involve many symmetry breaking structural fields and processes that occur at many time and length scales. We first present an account [1] of how the principles of coarse-graining in time and spatial domains can be used to develop realistic, material-specific models from first-principles quantum theoretical description of a material. Starting with accurate picture of chemical bonding in terms of electronic motion in a materials, these facilitate bridging of descriptions of a materials at multiple scales and capturing its temperature and pressure dependent structural phase transitions through statistical mechanical analysis with Monte Carlo (MC) and Molecular Dynamics (MD) simulations. We illustrate it with application to ferroelectric perovskite oxides and highlight (a) the insights obtained into microscopic mechanism of ferroelectricity, and (b) the errors or limitations that arise of the approximations used in density functional theory (DFT) [2]. We present generalization of this scheme of multi-scale modelling to challenging problems of Neel transition [3] with a giant magneto-elastic effect in multiferroic $YMnO_3$ and martensitic phase transformation [4] in NiTi shape memory alloys which have applications in actuator devices.

** Work done by Arpita Paul and Pawan Kumar, partly in collaboration with groups of John Perdew and Michael L Klein.*

Registration link for new participants: https://tinyurl.com/essya3me*

***participants who have registered for webinar#1 need not register again**

Zoom meeting details will be shared with the newly registered as well as earlier participants.

Conveners:

Dr. V.J.Surya and Dr.S. Yuvaraj

ACCMS-GRC Center-in-Charges

Department of Physics and Nanotechnology, SRMIST-KTR