ACCMS-Global Research Center
SRMIST, Chennai India

Webinar #19

Dr. Duc Nguyen Manh

Culham Centre for Fusion Energy, United Kingdom Atomic Authority, United Kingdom

Title: Toward finite-element modelling of hydrogen isotopes transport for fusion materials from first-principles calculations

Registration link: *https://tinyurl.com/2hy2urxr*
**Zoom details will be shared with the registered participants*

25 July 2023,
02.30 – 04.00 pm
Indian Standard Time

Short biography

Dr. Duc Nguyen-Manh is an academic researcher and senior scientist staff from United Kingdom Atomic Energy Authority. He is the principal investigator of 18 European Projects on Nuclear Fusion Materials, 14 International projects on High Performance computing, co-investigator of 8 international projects on computational materials science. He has Publish more than 200 papers in international journals in Physics, Chemistry, Materials and Engineering Sciences, Nuclear Materials, Computational Physics and Materials Science. His research interests are theory and modelling in physics, chemistry and engineering of materials, first-principles based electronic structure calculations; many-body problems in physics, multi-scale modelling in non-equilibrium systems, phase stability and transformation in nuclear materials, point defects and dislocation in materials under irradiation, and so on. He has been visiting scientist/OCAMAC fellow in University of Oxford, Visiting Professor at University Cergy-Pontoise, Paris, France, Visiting Scientist at University of Pennsylvania, USA, International Advisor Member of Key Lab. at VNU-HN, Visiting Professor at VNU-HCM, and Visiting scientist at Los Alamos National Laboratory, USA .

Abstract

Almost 30 years ago, we unraveled a materials modelling hierarchy involving research that spans the very broad spectrum of length scales from quantum mechanical calculations at the atomistic level all the way through to finite-element at the continuum level [1]. As a result, it provides valuable new insights into complex structures and their properties, opening the way to develop new computational materials science R&D activities together with improved process and product designs within the multiscale materials modelling scheme.

Fusion materials research with the technological challenges is intimately linked with the availability of suitable materials capable of reliably withstanding the extremely severe operational conditions of fusion reactors. Although fission and fusion materials exhibit common features, fusion materials research is broader. The harder mono-energetic spectrum associated with the deuterium–tritium fusion neutrons (14.1MeV compared to<2MeV on average for fission neutrons) releases significant amounts of hydrogen and helium as transmutation products that might lead to a (at present undetermined) degradation of structural materials after a few years of operation [2]. Therefore, a comprehensive understanding of the mechanisms of irradiation damage in condensed matter from multi-scale in time and space is essential for the development and optimization of advanced fusion materials. The damage and its evolution in time (nanoseconds to years) and space determines the macroscopic response of a material to irradiation and is thus crucial for understanding and predicting the evolution of the physical properties of structural and functional materials exposed to high fluences of fusion neutrons.

In this talk, a most recent and significant progress in theoretical development of theory of tritium transport in materials from first-principles calculations is presented with an emphasis on fusion application to entire reactor fuel cycles. The new modelling technique provides to overcome the big issue of uncertainty quantification of using classical McNabb Foster equations with empirical parameters and in the same time allows us to efficiently implement into finite-element modelling using Multi-physics Object-Oriented Simulation Environment (MOOSE) code.

Panelist

Prof. Bing-Joe Hwang,
National Taiwan University of Science and Technology, Taiwan

Convener:
Prof. Yoshiyuki Kawazoe
Head, ACCMS-GRC
SRMIST, KTR

Organizers:
Dr. V.J.Surya & Dr.S. Yuvaraj
ACCMS-GRC Center-in-Charges
Dept. of Physics and Nanotechnology, SRMIST, KTR

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