



Summer Workshop on “Modelling and Simulation in Materials Science and Engineering” with

Hands on Session (MSME 2018)

18-22 June, 2018

Organized by: Department of Physics (DST-FIST Sponsored),
Sathyabama Institute of Science and Technology
(Deemed to be University), Chennai-600119



ABOUT SATHYABAMA INSTITUTE OF SCIENCE AND TECHNOLOGY

Sathyabama University (A Christian Minority Institution) formerly known as Sathyabama Engineering College was established in 1987 by Dr. Jeppiaar. It is a premier institute imparting knowledge in the areas of engineering, science, technology and education. The University offers 27 programmes at UG level and 41 programmes at PG level in all disciplines. The University has excellent infrastructure facilities including modern laboratories, library with multimedia facilities, internet and other general amenities. University has written a special page in the history of space research on 22nd June, 2016 with the launch of “SATHYABAMASAT” in association with ISRO. The launch of “SATHYABAMASAT” and accolades received in world platforms is a specimen. Our motto is “TOGETHER FOR BETTER TOMORROW” and our mantra of Success is “LEARN TODAY and LEAD TOMORROW”. We practice and teach to our students that “JOY OF LIVING IS IN JOY OF GIVING”. The University aims to be the destiny of efficient and responsible technocrats those are fit enough to serve the industry and society.

ABOUT THE WORKSHOP

DFT codes in Computational Materials Science, allows to calculate the electronic structure of solids with high precision.

The goal of this course is:

- ◆ This Workshop is organized for the benefit of the PG students Researchers and faculties of Physics, Chemistry, Mechanical engineering and Nano technology to enlighten latest research developments of materials and their technological applications.
- ◆ The main objective of this workshop is to bring distinguished professors and renowned scientists to expose various developments in materials, address new challenges and solutions and also motivate them by interacting future research directions.
- ◆ To discuss how first-principles computational methods can drive the understanding, improvement and prediction of new technology based engineering materials and its application to material simulation
- ◆ Learn to utilize the codes like WIEN 2K and VASP and its application to simulate advance material for various applications.
- ◆ We start with detailed introductions and then have hands-on exercises with the WIEN2k/VASP program.

ABOUT DEPARTMENT OF PHYSICS (DST-FIST Sponsored)

Department of Physics was established in the year 1988. It offers courses in B.Sc., M.Sc., M.Phil., and Ph.D. The Department has been recognized as DST-FIST sponsored Department (2015-2020). The Department has excellent infrastructural facilities and other general amenities. The Department has undertaken various sponsored projects funded by such as **DST, DRDO and CARS for the worth of nearly 1.3 Crore**. We have organized international conference adoped by the visit of **Prof. Dr. Walter Kohn (Nobel Laureate-1998)** and video conferencing session by **Prof. Dr. Douglas Dean Osheroff (Nobel Laureate-1996)** in the year of 2014. The Faculties of the Department have expertise in various fields of research that includes Bulk, Thin film, Polymers & Nano Composite Materials, Crystal Growth and Characterization, Computational Materials Science and they have a strong technical background witnessed by their WoS/Scopus indexed research publications (91) with high impact factor.



TOPICS OF THE WORKSHOP

- ◆ Introduction to density functional theory
- ◆ Concepts of DFT codes for band structure calculations
- ◆ Structure optimization, building models with supercells, DFT+U
- ◆ Electronic, magnetic, optical, thermo electric, mechanical properties of various materials
- ◆ Use of the web-based graphical user interface (w2web) as well as the command-line interface
- ◆ “Hands-on” calculations with the WIEN2k /VASP code
- ◆ Discussions and exchange of experience between users.

ADVISORY COMMITTEE

1. Emeritus Prof. Dr. T. V. Rama Krishnan, BHU, IISc., Bangalore.
2. Prof. Dr. R. Asokamani, Secretary, The Academy of Sciences, Tamil Nadu.
3. Prof. Dr. M.Rajagopalan, CGC, Anna University (Retired).
4. Prof. Dr. Sushil Auluck, CSIR-NPL, IIT-Kanpur.
5. Prof. Dr. S. Mathi Jaya, IGCAR. MSG, Kalpakkam .

LECTURES & DEMO

1. Dr. Sushil Auluck, CSIR-NPL, IIT-Kanpur.
2. Dr. R. Asokamani, Secretary, The Academy of Sciences, Tamil Nadu
3. Dr. P. Ravindran, Professor , Central University of Tamil Nadu, Thiruvaur.
4. Dr. Vidya Ravindran, Dept of Medical Physics, Anna University.
5. Dr. V Subramanian, Sr. Principal Scientist, CSIR, Tamil Nadu.
6. Dr. E. Sampathkumaran, TIFR, Mumbai
7. Dr. Sharat Chandra, Scientist, MSG, IGCAR, Kalpakkam
8. Dr. C. Ravi, Scientific Officer, MSG, IGCAR, Kalpakkam.
9. Dr. Awadesh Mani, Scientific Officer. MSG, IGCAR, Kalpakkam.
10. Dr. B. R. K. Nanda, Asst. Professor, Dept. of Physics, IIT Madras.
11. Dr. Satyesh Kumar Yadav, Asst. Professor, Metallurgical and Materials Engineering, IIT Madras.
12. Dr. P. Murugan, Scientist, Functional Materials Division, CECRI, Karaikudi.
13. Dr. M. Victor Antony Raj, Asst. Professor, Loyola College, Chennai
14. Dr. I. B. Shameem Banu, Professor, B.S. Abdur Rahman Crescent Institute of Science and Technology, Chennai.
15. Dr. Pushpamithra, Scientist - E, Hindustan Institute of Technology and Science, Chennai.

HOW TO APPLY

Interested participants are requested to send the filled-in registration form and DD on or before **31-05-2018** to Email ID: wspmsms2018@gmail.com.

COURSE FEE:

Research scholar - Rs.2000 ; Faculty / Industry : Rs.2500

The registration amount is to be paid through DD with the name "Sathyabama Institute of Science and Technology" payable at Chennai.

Limited participants (40)

Participants are requested to bring their laptop for hands on training.

ACCOMMODATION

Limited accommodation will be provided on first come first serve basis.

ORGANIZING COMMITTEE

CHIEF PATRON

Tmt. Remibai Jappiaar,
Chancellor, Sathyabama Institute of Science and Technology.

PATRON

Dr. Marie Johnson, B.E., M.B.A., M.Phil., Ph.D.,
Vice President, Sathyabama Institute of Science and Technology.
Dr. Mariazeena Johnson, B.E., M.B.A., M.Phil., Ph.D.,
Pro Chancellor, Sathyabama Institute of Science and Technology.

ORGANIZING SECRETARY

Dr. M. Sundareswari,
Professor and Dean (School of Science and Humanities).

CONVENER

Dr. D. S. Jayalakshmi, Assistant Professor.

CO CONVENERS

1. **Dr. M. Manjula,** Assistant Professor.
2. **Mr. E. Viswanathan,** Research Scholar.

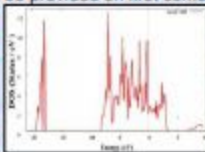
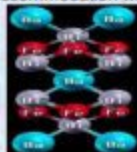
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Registration Form

1. Name of the candidate :
2. Designation :
3. Gender : Male / Female
4. Contact Number (Personal) :
5. Email ID :
6. Name of the College/Institution :
7. Payment Details Amount , bank, DD No. & date :
8. Whether Accommodation is required : Yes/ No

Date :

Signature of the Candidate



Address for Communication:
The Convener, MSME-2018,
Department of Physics (DST-FIST Sponsored)
Sathyabama Institute of Science and Technology,
Rajiv Gandhi Salai, OMR, Chennai-600 119.
Contact No.: 9840477004;9884973863

