## INTERNATIONAL E-WORKSHOP ON ELECTRONIC STRUCTURE THEORY AND APPLICATION TO CHEMICAL SYSTEMS



2<sup>nd</sup> - 6<sup>th</sup> November 2020



Organized by DEPARTMENT OF CHEMISTRY NATIONAL INSTITUTE OF TECHNOLOGY TIRUCHIRAPPALLI TAMIL NADU – 620015, INDIA

## **COORDINATORS**

Dr. L. Cindrella, Professor (HAG) & Dean(FW)

Dr. V. M. Biju, Associate Professor & Associate Dean (FW)

Dr. A. Sreekanth, Associate Professor

Dr. Sunandan Sarkar, Assistant Professor

### **ABOUT THE INSTITUTE**

The National Institute of Technology Tiruchirappalli, situated in the heart of Tamil Nadu was started as a joint and cooperative venture of the Government of India and the Government of Tamil Nadu in 1964 with a view for catering to the needs of man-power in technology for the Country. NIT Tiruchirappalli is one of the 31 NITs established by the Government of India. The Institute retained its No.1 position among all NITs and ranked 9<sup>th</sup> in Engineering in the "India Rankings 2020" released by NIRF, MHRD Government of India. The Institute offers UG Courses in ten branches and PG Courses in twenty-one disciplines of Science, Engineering & Technology besides M.S. (by Research) and Ph.D. in all the departments.

### **ABOUT THE DEPARTMENT**

The Department of Chemistry has a long history of providing PG course in general Chemistry and research program in frontier areas of Chemistry. It has acquired the state of art research facilities, sophisticated instruments and well equipped laboratories. The Department is committed to high quality academic programmes and cutting edge research programmes. The Department has been consistently receiving research funds from various funding agencies like MHRD, CSIR, BRNS, DRDO, DST etc.

### SCOPE OF THE WORKSHOP

This workshop aims to motivate the students in the field of computational modeling and simulation, and to provide a future direction to eco-friendly and cost-effective research in designing efficient materials for energy and biological applications. The electures will be presented by experienced Professors and Scientists from India and Abroad. The participants will learn computational aspects of quantum theory and machine learning approaches. The Faculty members, scholars and students from the academic Institutions/ Research Labs are eligible to attend.

#### **MODE** Online Video Conferencing

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**Dr. Swapan K Ghosh** Distinguished Professor, Department of Atomic Energy, University of Mumbai



Dr. Sourav Pal Director and Professor, Department of Chemical Sciences, IISER-Kolkata

Dr. Prasad V Bharatam Professor, Department of Medicinal Chemistry, NIPER-Mohali



**Dr. Swapan K Pati** Professor & Chairman, Theoretical Sciences Unit, JNCASR, Bangalore



**Dr. Pranab Sarkar** Professor, Department of Chemistry, Visva-Bharati, Santiniketan

Dr. Raghavan B Sunoj Professor, Department of Chemistry, IIT-Bombay



**Dr. Ayan Datta** Professor, School of Chemical Sciences, IACS, Kolkata



**Dr. Suresh C H** Senior Principal Scientist, CSIR-NIIST, Trivandrum



Dr. Yihan Shao Assistant Professor, Department of Chemistry & Biochemistry, University of Oklahoma, USA



Dr. Barry D Dunietz Associate Professor, Department of Chemistry & Biochemistry, Kent State University, USA



**Dr. Michal Otyepka** Deputy Director, Professor, RCPTM, Department of Physical Chemistry, Palacký University, Czech Republic

# **REGISTRATION** (Due Date: 31-10-2020)

Registration fees for Students: Rs. 300/-, Research Scholars/Postdocs: Rs.400/and Faculty Members: Rs.500/-

Registration fee shall be paid to the following account through NEFT/IMPS:
Account Name: The Director, NIT, Tiruchirappalli
Account No: 10023883064
IFSC Code: SBIN0001617
Payable at: State Bank of India, NIT, Trichy

After the payment of the registration fee, Confirm your registration by uploading the image of the payment proof through the following link: <u>https://forms.gle/h2mVsmqvPSLDDT8E9</u>

We will share the **programme details** and **meeting link** to the registered Participants.

For any clarification please contact us: (+91) 9443843076, (+91) 9153484492