



**SATHYABAMA UNIVERSITY**  
(Established under Section 3 of UGC Act, 1956)  
Declared as Category A University by MHRD, Govt. of India  
Jeppiaar Nagar, Rajiv Gandhi Salai, Chennai - 600119



## DEPARTMENT OF CHEMISTRY

*Cordially invites you to the **DST-SERB**  
sponsored five day workshop on  
“**CHALLENGES AND ADVANCES  
IN COMPUTATIONAL  
CHEMISTRY CACCh-2018**”*

To be held from 08-January-2018 to 12-January-2018 at  
**SATHYABAMA UNIVERSITY**  
VENUE: Admin Block Auditorium



### ABOUT SATHYABAMA UNIVERSITY

Sathyabama University is a pioneer in Engineering Education and was established with the aim of providing quality higher education in the areas of Engineering, Science and Technology on par with International standards. It persistently seeks and adopts innovative methods to improve the quality of higher education on a consistent basis. Having acquired excellence in the academic part of education with all sophisticated facilities available, the University has established several research centres in the field of Remote Sensing & Geo Informatics, Nano Technology, Ocean Research, Water Research, Robotics, Earth & Atmospheric Sciences, Non Destructive Testing & Waste Management in collaborations with esteemed National Research organizations and are progressively working towards innovation in the field of Science & Technology. The University has been accredited with 'A' grade by National Assessment and Accreditation Council (NAAC) and ISO 9001: 2008 Certification for Professional Quality Management Practices. The University has undertaken various Sponsored and Collaborative Research and Development projects funded by national organizations such as Indian Space Research Organization (ISRO), Department of Science and Technology (DST), Indira Gandhi Centre for Atomic Research (IGCAR), Defence Research and Development Organization (DRDO), Department of Bio-Technology (DBT), Ministry of Environment and Forests (MoEF), Board of Research in Nuclear Sciences (BRNS) etc., The University holds great promise to expand the applications of space technology, benefiting the common man and enriching the quality of life. A step towards achieving this, the University is successfully conducting non formal education programmes through 18 Village Resources Centre (VRCs) all over the state of Tamil Nadu.

### ABOUT THE DEPARTMENT OF CHEMISTRY

The department of chemistry was started right from the inception of University in the year 1988. It has well-established laboratories equipped with sophisticated instruments, which fulfil the needs of PG and Ph. D students. The department has highly qualified faculty and more than 20 Ph. D students. It has 12 doctorates from reputed institutions like IIT, NIT CEERI, NML, etc. and published more than 75 research papers in reputed journals with high impact factor. The department has undertaken many research projects funded by CSIR, ISRO, DST and IGCAR.

### NATIONAL ADVISORY COMMITTEE

Dr. Rajaraman, Associate Professor, IIT Bombay  
Dr. Gunasekaran K, Associate Professor, University of Madras  
Dr. Narahari Sastry G, Sr. Principal Scientist, Centre for Molecular Modelling, CSIR-IICT, Hyderabad.  
Dr. Naresh Kandakarla, Manager R&D & Production at Helios Bio Nutrition Pvt. Ltd.  
Dr. Geetha Swaminathan, Former Vice Principal, Stella Maris College, Chennai.  
Dr. K. Shyamala, Former Head, Department of Bioinformatics, Stella Maris College  
Dr. R. Karvembu, Associate Professor, Department of Chemistry, NIT Trichy  
Dr. A. Nityananda Shetty, Professor, NITK, Suratkal

### OBJECTIVES AND IMPORTANCE OF THE WORKSHOP CACCh-2018

Chemists have been involved in computations for ages, but what we know as Computational Chemistry” is a product of the digital age. However, Computational Chemistry did not come into its own until 1998 when Walter Kohn and John Pople won the Nobel Prize for Chemistry for their work in Density Functional Theory and Computational methods in Quantum Chemistry. It is rapidly growing field of Chemistry and is now firmly established as an indispensable tool in the hands of researchers to carry out studies hitherto unachievable by conventional methodologies. This interesting field of study helps to create spectral profile simulations, modelling and designing molecules, understand structure activity relationships, homology modelling, design more productive and efficient processes, protein structure visualization, in molecular dynamics and in short to extract useful knowledge from oceans of data.

To bring about a better understanding of the scope of Computational Chemistry and its application in current research and education by UG and PG students and teachers, research scholars, etc, the Department of Chemistry has organized a five day Workshop on the Challenges and Advances in Computational Chemistry 2018 (CACCh-2018) that will focus on the molecular mechanism underlying human health and disease. This workshop will provide a comprehensive theoretical and practical hands-on training to all the participants on molecular modelling and drug design.

#### CONVENER

Ms. JANET SABINA X  
Assistant Professor  
Department of Chemistry  
Sathyabama University  
Rajiv Gandhi Salai  
Chennai – 600119

REGISTRATION FEE: RS. 2000.

Kindly confirm your participation through phone or email. Registration through SMS to 9445362213.

Email: [janetjeyakumar@gmail.com](mailto:janetjeyakumar@gmail.com)

#### LIST OF SPEAKERS

Dr. Narahari Sastry G, CSIR-IICT, Hyderabad

Dr. Athi Naganathan, IIT Madras

Dr. Rajaraman, IIT Bombay

Dr. Gunasekaran, Madras University

Dr. Xavier Suresh, Sathyabama University

Dr. Deva Priyakumar, IIIT Hyderabad

Dr. Mukesh Doble, IIT Madras

Dr. Naresh Kandakatla, Manager, Helios Bio Nutrition Pvt. Ltd.

Dr. Xavier Suresh, Sathyabama University

Dr. Naresh Kandakatla, Manager, Helios Bio Nutrition Pvt. Ltd.

Dr. Thiyagarajan, IBAB, Bangalore

#### HIGHLIGHTS

- Eminent scientists from IIT Madras, Bombay, IICT Hyderabad and the industry will deliver talks on various topics in Computational Chemistry
- Practical sessions and interactive session with eminent personalities
- A highly comprehensive five day programme that will enrich all researchers in this field.