

## About the workshop

This workshop will provide hands-on-training in *Computational Chemistry* tools relevant for theoretical studies of materials. The speakers are from a range of fields such as Molecular Dynamics, Density Functional Theory, *ab initio* methods, Programming Language (FORTRAN & PYTHON), Chemical biology and High-Performance Computing. The department of Chemistry at J. C. Bose University of Science and Technology, YMCA will be hosting the workshop in Online mode.

## Aim/Objective

- To develop awareness of basic theoretical and computational chemistry
- To be familiar with various applications of computational chemistry
- To get a hands-on training on specific computational chemistry tools

## Resource Person

### Keynote Speaker

- **Prof. Balasubramanian Sundaram**  
*CPMU, JNCASR Bangalore*

### Hands-On Training

- **Dr. Sairam Swaroop Mallajosyula**  
*IIT Gandhinagar*
- **Dr. Sandeep Kumar Reddy**  
*IIT Kharagpur*
- **Dr. Koushik Mondal**  
*IIT (ISM) Dhanbad*
- **Dr. Anuj Kumar Sharma**  
*Central University of Rajasthan*
- **Dr. Avinash**  
*BHU Varanasi*
- **Dr. Mahesh Sundararajan**  
*BARC Mumbai*
- **Dr. Vinod Kumar**  
*JCBOSEUST, YMCA Faridabad*

### Patron-in-Chief

**Prof. Dinesh Kumar**

Vice-Chancellor,

J. C. Bose University of Science & Technology, YMCA

### Patron

**Dr. Sunil Kumar Garg**

Registrar,

J. C. Bose University of Science & Technology, YMCA

### Chief-Guest

**Prof. Lalit Kumar Awasthi**

Director

**Dr. B. R. Ambedkar NIT - Jalandhar**

### Program Advisor

**Prof. Ashutosh Dixit**

Dean, Faculty of Sciences

J. C. Bose University of Science & Technology, YMCA

### Program Chair

**Dr. Ravi Kumar**

Chairman, Department of Chemistry

J. C. Bose University of Science & Technology, YMCA

### Convener

**Dr. Anurag Prakash Sunda**

Assistant Professor, Chemistry

J. C. Bose University of Science & Technology, YMCA

### Sponsored By:

J. C. BOSE UNIVERSITY OF SCIENCE & TECHNOLOGY,  
YMCA

## One Week Online National e-Workshop

on

## HANDS-ON TRAINING & PRACTICES IN

## COMPUTATIONAL CHEMISTRY

November 23-27, 2020

Organized By:



DEPARTMENT OF CHEMISTRY

J. C. BOSE UNIVERSITY OF SCIENCE &  
TECHNOLOGY, YMCA

Faridabad 121006



## Workshop Topics

### Keynote Lecture:

- *Molecular Modelling & Simulations of Materials* by Prof. Balasubramanian Sundaram

### ACM Distinguished Speakers Program (DSP)

- *Data Mining and Data Analysis Applications with R/Python* by Dr. Koushik Mondal (Approved by ACM)

### Training Sessions

- *Forcefields and applications* by Dr. Sairam
- *Numerical methods and Geometry Optimization* by Dr. Sandeep K Reddy
- *UV Data Processing using SCAN and NOVA Software tools for voltammograms* by Dr. Anuj Kumar Sharma
- *Fortran Programming* by Dr. Avinash
- *DFT: Tutorials using ORCA software & Gabedit* by Dr. Mahesh Sundararajan
- $\Sigma$ SIGMAPLOT: *Graphics* by Dr. Vinod Kumar
- *VMD, Z-Matrix Construction using MOLDEN and L<sup>A</sup>T<sub>E</sub>X Scientific Writing using T<sub>E</sub>XMAKER* by Dr. Anurag

### Free Sponsored Training Session:

CHEMDRAW: *Chemical Structure Drawing* by M/S. SCUBE Software Solution Pvt Ltd., New Delhi



## Schedule

### 23.11.2020 Day - ①

- 10.30 AM Inaugural by Hon'ble Vice-Chancellor
- 10.45 AM Inaugural Address by the Chief Guest
- 11.35 AM Keynote Lecture
- 01.30 PM Lunch Break
- 02.30 PM Training Session-1: Force-Field

### 24.11.2020 Day - ②

- 10.00 AM Training Session-2: Numerical methods & Geometry Optimization
- 01.00 PM Lunch Break
- 02.00 PM Training Session-3: Z-matrix constructions in MOLDEN & Coordinate File Formats

### 25.11.2020 Day - ③

- 10.00 AM Training Session-4: Data Mining & Data Analysis with R/Python
- 12.00 PM Training Session-5: Fortran Programming
- 01.00 PM Lunch Break
- 02.00 PM Training Session-6: VMD & GRACE

### 26.11.2020 Day - ④

- 10.00 AM Training Session-7: Data Processing SCAN & NOVA Software tools
- 11.30 AM Training Session-8: CHEMDRAW
- 01.00 PM Lunch Break
- 02.00 PM Training Session-9: VMD & GRACE

### 27.11.2020 Day - ⑤

- 10.00 AM DFT: Basics and Applications
- 11.00 AM Training Session-10: DFT Tutorials ORCA software & Gabedit
- 01.00 PM Lunch Break
- 02.00 PM Training Session-11:  $\Sigma$ SIGMAPLOT
- 04.00 PM Valedictory Session

## Registration

Registration Mode: Online

[Click Here](#)

### Registration Fee\*:

For Student - Rs. 500/- & For Faculty - Rs. 1000/-

**Start Date** of Registration: Oct 15, 2020

**Last Date** of Registration: Nov 15, 2020

### Limited seats

Short-listed Participants will be intimated through mail for fee payment and Online meeting link (ID). The last date of registration fee payment is 18<sup>th</sup> November 2020.

\*Registration Fee is not applicable for **host department** students.

### Bank Account Details:

Account Name: J. C. BOSE UST YMCA Faridabad

Bank: Indian Overseas Bank YMCA

A/c No: 146601000000088

IFSc Code: IOBA0001466

MICR Code: 110020044

## Contact Us

Preferred Contact Hrs: 4 - 5 PM

### Organizer:

**Dr. Anurag Prakash Sunda**

Assistant Professor, Chemistry

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### Student Volunteers:

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