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:

One Week Online 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
  (Approval Pending from 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 Sundaranjan
• ΣSIGMA PLOT: Graphics by Dr. Vinod Kumar
• VMD, Z-Matrix Construction using MOLDEN and LaTeX Scientific Writing using TeXMaker by Dr. Anurag

Free Sponsored Training Session:
CHEMDRAW: Chemical Structure Drawing by M/S. SCUBE Software Solution Pvt Ltd., New Delhi

Schedule

<table>
<thead>
<tr>
<th>Date</th>
<th>Time</th>
<th>Session</th>
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<tbody>
<tr>
<td>23.11.2020</td>
<td>10.30 AM</td>
<td>Inaugural by Hon’ble Vice-Chancellor</td>
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<td>10.45 AM</td>
<td>Inaugural Address by the Chief Guest</td>
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<td>11.35 AM</td>
<td>Keynote Lecture</td>
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<td>01.30 PM</td>
<td>Lunch Break</td>
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<td>02.30 PM</td>
<td>Training Session-1: Force-Field</td>
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<tr>
<td>24.11.2020</td>
<td>10.00 AM</td>
<td>Training Session-2: Numerical methods &amp; Geometry Optimization</td>
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<td>01.00 PM</td>
<td>Lunch Break</td>
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<td>02.00 PM</td>
<td>Training Session-3: Z-matrix constructions in MOLDEN &amp; Coordinate File Formats</td>
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<tr>
<td>25.11.2020</td>
<td>10.00 AM</td>
<td>Training Session-4: Data Mining &amp; Data Analysis with R/Python</td>
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<td>12.00 PM</td>
<td>Training Session-5: Fortran Programming</td>
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<td>01.00 PM</td>
<td>Lunch Break</td>
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<td>02.00 PM</td>
<td>Training Session-6: VMD &amp; GRACE</td>
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<tr>
<td>26.11.2020</td>
<td>10.00 AM</td>
<td>Training Session-7: Data Processing SCAN &amp; NOVA Software tools</td>
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<td>11.30 AM</td>
<td>Training Session-8: CHEMDRAW</td>
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<td>01.00 PM</td>
<td>Lunch Break</td>
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<td>02.00 PM</td>
<td>Training Session-9: VMD &amp; GRACE</td>
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<tr>
<td>27.11.2020</td>
<td>10.00 AM</td>
<td>DFT: Basics and Applications</td>
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<td>11.00 AM</td>
<td>Training Session-10: DFT Tutorials ORCA software &amp; Gabedit</td>
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<td>01.00 PM</td>
<td>Lunch Break</td>
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<td>02.00 PM</td>
<td>Training Session-11: ΣSIGMA PLOT</td>
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<td>04.00 PM</td>
<td>Valedictory Session</td>
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Registration

Registration Mode: Online

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 18th November 2020.

*Registration Fee is not applicable for host department participants.

Bank Account Details:
Account Name:
Bank: Indian Overseas Bank YMCA
A/c No:
IFSC Code:
MICR Code:

Contact Us
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Organizer:
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J. C. Bose University of Science & Technology, YMCA, Faridabad 121006
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