

ABOUT THE INSTITUTE

Sardar Vallabhbhai National Institute of Technology (SVNIT), is one of the thirty one National Institutes of Technology in India. The Institute campus is spread over 100 hectares of land on the Surat-Dumas Road.



The Institute was established in 1961 in Gujarat State as a Regional Engineering College (REC). The same became National Institute of Technology (NIT) in, 2002. In the year 2021, the institute celebrated its Diamond Jubilee year.

At present, the institute is offering 6 UG Programmes, 18 PG Programmes and Five Years Integrated M.Sc. (Chemistry, Physics & Mathematics) including doctoral programme in all the above branches with an objective to impart high quality technical education to meet the global needs in the present competitive world. The National Institutional Ranking Framework (NIRF) of the Ministry of Education Government of India, has identified SVNIT as one of the best Institute of National importance of Government of India. All departments are well furnished with research facilities.

ABOUT THE DEPARTMENT

The Department of Chemistry established in 1961-62, is a dynamic multidisciplinary center engaged in all fields of Chemical Sciences. The Department offers Five Years Integrated M.Sc. in Chemistry and Ph.D. programme in multidisciplinary research areas.

The department has 14 qualified and dedicated faculty members. The department is comprehended for its interdisciplinary research covering Materials Science, Biomaterials, Nanomaterials, Computational chemistry, Organic Synthesis, Catalysis, Polymers, Chemosensors, Supramolecular Chemistry, Deep Eutectic Solvents, Green Chemistry, Solution Chemistry, Waste Water treatment etc. The department is credited with various research funding agencies like DST, BRNS, UGC-DAE, CSIR, GUJCOST, etc.

ABOUT THE STTP

The STTP will provide the participants from the academic and research institutes to work with quantum mechanical and visualization softwares, such as **Gaussian**, **Multiwfn**, **chemcraft**. Researchers working on the various fields of chemistry with no prior knowledge of these softwares can join this STTP. All demonstrations will be given at computational facility of the Department of Chemistry, SVNIT in the offline mode only. This STTP aims to share the fundamental/basic knowledge to the participants required before entering into the computational chemistry field. Also, the step-wise calculations, data collection for publication and interpretation will be discussed. Within five days, the following topics will be covered:

- Introduction to computational chemistry (Quantum and Molecular Mechanical Calculations)
- DFT calculations in Gaussian (Basis Sets and functionals)
- Single-Point Energy & Geometry Optimization
- IR and Raman spectra calculations
- UV-Vis and NMR spectra calculations
- Thermochemistry
- Working with Multiwfn
- Training on various visualization softwares

SHORT TERM TRAINING PROGRAMME

Computational Chemistry: Methods and Techniques for Beginners (CCMTB - 2023)

28th Feb-4th March 2023

ORGANIZED BY



**Department of Chemistry,
Sardar Vallabhbhai
National Institute of Technology (SVNIT)
Surat – 395 007, Gujarat, India**

COORDINATORS

**Dr. Suban K. Sahoo, Associate Professor
Dr. Arup K. Ghosh, Assistant Professor**

In association with:

CCE, SVNIT.



ABOUT SURAT CITY

Surat, historically known as *Suryapur*, is a port city situated on the bank of the Tapti river. This beautiful city is well known for textiles, zari and diamonds along with several large scale industrial units. Important tourist places in Surat include The Dutch garden, Tithal beach, Suvali beach, Surat castle, among many more attractions.

CLIMATE

The last week of Feb and first week of March is the time of retreating winter in Surat. Hence, the weather is pleasant with expected temperatures ~ 24-30° C.



ADDRESS FOR CORRESPONDENCE

Dr. Arup K. Ghosh (M): 9073060145
Dr. Suban K. Sahoo (M): 9265893477

DEPARTMENT OF CHEMISTRY
SARDAR VALLABHBHAI NATIONAL
INSTITUTE OF TECHNOLOGY (SVNIT),
SURAT – 395 007, GUJARAT, INDIA
Email: ccmtb2023svnit@gmail.com

REGISTRATION DETAILS

The registration fees,

- For PG / Research Students: **Rs. 1770/-**
 - For Faculty members: **Rs. 2950/-**
 - For Industry delegates: **Rs. 5900/-**
- Registration fees are inclusive of GST@ 18%
- **Accommodation available for limited number of participants on payment basis.**
 - **Meals may arranged by the participant at their own cost from SVNIT canteen located just beside the department of chemistry.**

• **Last date for Registration: 20/02/2023.**

- The participants should pay the registration fees by online transfer only to the account as detailed below.

Bank Name: State Bank of India

Account No.: 37030749143

Account Name: Director, SVNIT-CCE

Nature of Bank: Current Account

IFSC Code: SBIN0003320

Swift Code: SBININBB

Brach Code: 03320

Bank Branch: SVRCET, Surat

SCAN & PAY



- The participants should get registered using following registration link –

• https://forms.gle/EJ8xwQBmC7cWZs_kF6

- Certificates will be issued to all registered participants.

• **Note: The maximum number of participants is limited to 30** and the registration will be on first come first serve basis.

ORGANIZING COMMITTEE

CHIEF PATRON:

Prof. Anupam Shukla,
Director, SVNIT, Surat

CHAIR:

Dr. Suresh Kumar,
Head, DoC, SVNIT, Surat

COORDINATORS:



Dr. Suban K. Sahoo
Associate Professor,
DoC, SVNIT.



Dr. Arup K. Ghosh
Assistant Professor,
DoC, SVNIT.