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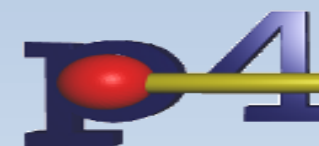
2nd Hands on Training on Multiscale Simulation in Advanced Materials Science & Technology (HTMSAMST-2023)

10-14 June 2023

Organized By



Department of Physics
Sardar Vallabhbhai National Institute
of Technology (SVNIT), Surat



ABOUT THE WORKSHOP

The discovery of new material highly impacts the technological development. Computational tools play an important role in such findings. One of the most reliable computational tool is density functional theory (DFT). The aim of this workshop is to cover basic concepts DFT. Apart from the consideration of standard tasks implemented in most ab-initio codes, such as how to calculate the electronic (band) structure, perform structure (geometry) relaxation, calculate lattice vibrations or run molecular dynamics simulations, the specific topics to be covered include the generation and use of pseudopotentials, the construction of basis sets of strictly localized numerical atomic orbitals, and basic notions about the efficient computation of the matrix elements with linear scaling methods and the role the real-space grid.

Quantum Espresso and SIESTA are an open source software based on DFT. TansSiesta is used to study the transport properties of materials. Xcrysden and P4VASP are visualization software. The workshop will give an insight into working principle of Quantum Espresso, SIESTA and TranSiesta.

TOPICS COVERED

- Basics of Linux programming
- Installation & Hands on session on P4VASP, Xcrysden
- Basics of density functional theory
- Installation & Hands on session on Quantum Espresso
- Installation & Hands on session on Siesta and TranSiesta
- Generations of pseudopotentials: vdW, HSE
- Structural, Electronic, Phonon, Transport properties
- Optical and different executable for plotting
- Interactive sessions: Panel discussions

REGISTRATION DETAILS

Research Scholars	Rs. 3,540/- (Including 18% GST)
Faculty Member	Rs. 4,720/- (Including 18% GST)
Industry Person	Rs. 5,900/- (Including 18% GST)

Registration fee includes registration kit, working lunch and course materials. **The only selected participants (limited to 30 persons) need to pay registration fees.** The participants have to bear their own travelling expenses. The accommodation can be arranged upon prior request on payment basis in the Narmad Bhavan Guest House. Research scholars have to attach photocopy of their valid identity card along with registration form. Registration Form Link [[PDF](#)]

The non-refundable registration fees should be sent through internet (NEFT). Bank details for online transfer of registration fees:

Bank Account Name: Director, SVNIT-CCE

SBI Account No.: 37030749143

Bank Name: State Bank of India

IFCS Code: SBIN0003320

Branch: SVRCET Branch.



IMPORTANT INSTRUCTIONS

- The last date of registration is 30 May, 2023.
- The selected applicants will be intimated by 2 June 2023 by e-mail.
- Spot registration may be permitted in case of available vacancies.

CONTACT PERSON

Dr. Yogesh Sonvane

Department of Physics,

Sardar Vallabhbhai National Institute of Technology, Surat,
Gujarat, India

Email: yas@phy.svnit.ac.in