

3-DAY WORKSHOP ON

DFT:

APPLICATIONS IN COMPUTATIONAL MATERIALS SCIENCE



VIT®

Vellore Institute of Technology

(Deemed to be University under section 3 of UGC Act, 1956)

VIT VELLORE



THREE DAYS



HANDS-ON
SESSIONS



EXPERT
LECTURES



POSTER
SESSIONS



September 28 – 30, 2026



VIT, Vellore – 632014, Tamil Nadu, India



Open to: Students, Researchers,
and Faculty



70 Seats Available



Register before
14th SEPTEMBER 2026



LECTURE TOPICS

- Early Density Models and Foundations
- Hohenberg–Kohn Theorems and Formalism
- Exchange–Correlation Functionals
- Plane-Wave Basis Sets and k-Point Sampling
- Pseudopotential Theory and Projector Augmented Wave (PAW) Method
- Structural Relaxation and Geometry Optimization
- Density Functional Theory for Magnetism and Spintronics
- First-Principles Design of Quantum Materials
- Magnetism in 2D Materials
- Applications of DFT in Quantum Materials and Topological Systems
- Applications of DFT in Energy Storage



HANDS-ON TRAINING

- Structural Optimization of Bulk and 2D Materials
- Band Structure and DOS calculations
- Phonon calculations
- Surface Energy Calculations
- Computational descriptors for energy storage materials



REGISTRATION FEES

PhD Scholars	: ₹2000
Postdoctoral Researchers	: ₹2500
Faculty	: ₹3000



Refreshments and lunch are included with the registration fees.



Accommodation has to be booked separately inside the students hostel.



Preference will be given to first cum first serve basis.



CONFIRMED LIST OF SPEAKERS

1. **Prof. Ranjit Thapa**
SRM University-AP, Andhra Pradesh
2. **Dr. Sooraj Kunnikuruvan**
IIT Madras
3. **Dr. Chaitanya Sharma Yamijala**
IIT Madras
4. **Dr. Hrishit Banerjee**
University of Dundee, England
5. **Prof. Saswata Bhattacharya**
IIT Delhi
6. **Dr. Sayantika Bhowal**
IIT Bombay
7. **Dr. Tanay Nag**
BITS Pilani, Hyderabad Campus
8. **Dr. Banasree Sadhukan**
Mahindra University, Hyderabad



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ORGANIZED BY:

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