1ST ONLINE HANDS-ON-TRAINING ON

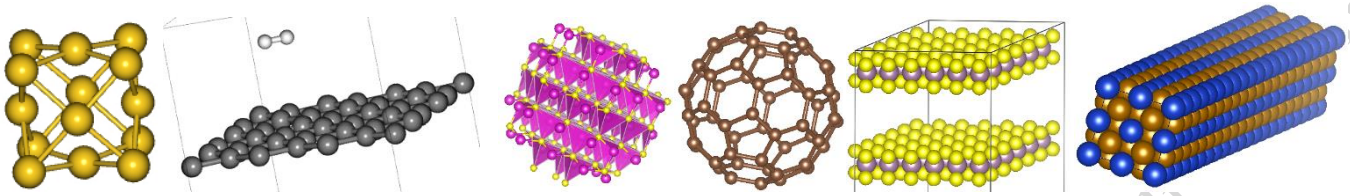
DENSITY FUNCTIONAL THEORY OF ADVANCED MATERIALS

(USING QUANTUM ESPRESSO PACKAGE)

Centre for Advanced Computational Research, New Delhi, India

(Registered under Ministry of SME, Government of India for Research and Experimental Development on Natural Sciences and Engineering)
(ISO 9001:2015 Certification for Hands-on-Training on Computational Science including DFT calculation of Materials, Molecular Docking and Dynamics)

Website: https://cacrdelhi.com, Email: admin@trainingcacrdelhi.com



Date: 25th Feb. – 6th Mar. 2025

Timing: Morning Batch: 9:00 AM – 10:00 AM IST or Evening Batch: 9:00 PM – 10:00 PM IST

[Online Live Sessions along with Complete Recordings]

1. FDP/Workshop (Hands-on-Training) Program: Batch 2

We are glad to announce next **10-Days Online FDP/Workshop (Hands-on-Training) program on DFT Modelling of Advanced Materials [DFT-Advanced] (Hands-on-Training using Free Licence Software Tools: Quantum Espresso & Vesta)**.

- In recent years, major scientific and industrial interest has been attracted in the multiscale structures involving nanoparticles, thin films, monolayers, etc and their structure–property relationships. The need for such novel materials demands the understanding of the changes in structural and dynamical properties caused at the microscopic level.
- Electronic structure calculations from Density functional theory (DFT) are a well-established approach for predicting a large range of material properties. Not surprisingly, many advances have been made in theoretical models and simulation approaches to predict electronic structure, optical behaviour, magnetic & mechanical properties.

2. Please visit below webpage and submit your Registration Form and Fees

https://www.cacrdelhi.com/upcomingsession

or

https://www.cacrdelhi.com/event-details/10-days-online-fdp-workshop-on-dft-modelling-of-materials-advanced-hands-on-training-4

Note: Those registering for the Advanced Training Session are requested to complete the Basic Training from our **YouTube Playlist**.

YouTube

Join our WhatsApp Group

3. Detailed Daywise Schedule

Part A: System Designing and Modelling using Vesta Software Package		
	In Session (Live)	Practice (HW)
25 Feb. 2025: **Session 1**	Nanocrystal (1-100 nm) 1. CdSe: Cation and Anion rich Structural Designing 2. Gold (variable sizes): Spherical Shape Structural Designing Quantum Dot (0.1 – 10 nm) 1. Graphite QD Structural Designing 1. Copper QD Structural Designing	
26 Feb. 2025: **Session 2**	Monolayer (2D Structure) 1. Gold Monolayer Structural Designing 2. VSe_2 Monolayer Structural Designing	1. $PtSe_2$
	Multilayer 1. Bi_2Se_3 Bilayer Structural Designing 2. CdSe 4 layers Structural Designing	1. V_2O_5 Bilayer 2. Pt 8 Layers
27 Feb. 2025: **Session 3**	Nanowire 1. Gold (aspect ratio >1000) nanowire Structural Designing 2. Pt/Pd Core-Shell nanowire Structural Designing	1. TiO_2
28 Feb. 2025: **Session 4**	Heterostructures (Part 1) 1. Gold NanoCrystal / Graphene Monolayer 2. Graphene /C_{60}	1. CdI_2 / Graphene
Part B: Properties Investigation using Quantum Espresso		
1 Mar. 2025: **Session 5**	▪ Pseudopotentials, Parametrization: plane wave function, kinetic energy & charge density cut-off ▪ Selection of high symmetry points for SCF ▪ Self-Consistent Field (SCF) calculation ▪ Calculation of BAND-GAP from SCF calculation	
2 Mar. 2025: **Session 6**	**Band gap computations for:** 1. Si unit cell structure 2. n-type and p-type semiconductors 3. Ionic crystals: $BaAl_2O_4$ etc. 4. Organic materials: Pentacene etc. 5. Nanoparticles: Au, Ag, MoS_2 etc.	
3 Mar. 2025: **Session 7**	▪ DFT Structural optimization (relax and VC-relax): doped unit cell, ionic crystals, nanocluster, monolayer ▪ **Optical properties calculation:** Band Structure (E vs. K: Dispersion curves) Calculations for conductors, semiconductors & insulators ▪ Band Gap, **Direct vs Indirect Semiconductors**, Density of States (DOS), ▪ Spin polarised **Magnetic Moment** calculation ▪ Calculation on **NANOCLUSTER** DFT code	
4 Mar. 2025: **Session 8**	Photovoltaic Studies ▪ Electrical Conductivity: Effective Mass Calculation, Electronic Mobility ▪ Partial Density of States Calculation, Orbital contribution	
5 Mar. 2025: **Session 9**	Non-covalent Interaction ▪ Adsorption and Interaction Studies ▪ Molecular Dynamics (MD) Study, Vibrational modes	
6 Mar. 2025: **Session 10**	▪ Simulate Powder XRD PATTERN using VESTA ▪ Concluding Remarks	

4. Salient Features

- ✓ The Hands-on-training Program is planned for **Faculty** (**FDP Completion Certificate**) and **Post-docs, Research Scholars, post-graduate students (Certification of Training completion).**
- ✓ Training Session is designed as per the guidelines defined by the UGC and can be used for Research Articles publication.
- ✓ The **links to download the required free software's for training will be provided**. We understand the Academic schedules of participants so **complete lecture recordings** will be given to all participants.
- ✓ Hands-on-Training sessions will be taken via online mode, Lecture Mode: English
- ✓ e-certificates will be provided to all registered participants (**subjected to minimum 4/10 attendance as per UGC guidelines**)
- ✓ Training will be provided on Windows Operating system
- ✓ Programming and coding knowledge is **not required** for above Hands-on-Training.
- ✓ On successful Registration, an automated email will be sent to confirm your participation.

5. Registration Category and Fees

Registration Type	National
Post-doctorate's Participants	Rs. 2,000
Research Scholars Participants	Rs. 1,500
Undergrad and Postgraduate Students	Rs. 1,000
Faculty	Rs. 2,500

Contact at:
admin@trainingcacrdelhi.com, nikhilaggarwal@alumni.iitm.ac.in
+91 9790969349 via call or WhatsApp message for any query.

6. About Us

Centre for Advanced Computational Research, New Delhi, India, established in April 2021, is an International Research unit with research focus in Materials Sciences, Analytical chemistry, Organic & Inorganic chemicals synthesis, Pharmaceuticals and Bioinformatics. The R&D activities primarily involve the in-depth spectroscopic studies of Novel material via modern computational chemistry/physics approaches toward their applications in organic light-emitting diodes (OLEDs), Photovoltaics, catalysis, Optoelectronic devices, polymer design, energy-based materials, non-linear optical activity, energy transfer mechanisms, and Bioinformatics. The organization is headed by Dr. Nikhil Aggarwal along with 15 External Faculty Members and 18 project students from the premier research institutions of India and abroad including IISC Bangalore, IITs, NITs, CSIR Labs, etc. We are proud to say that our faculty members are actively engaged in frontier research projects and has concrete research publications. The Centre has successfully installed two powerful workstations to enhance research activities. We are also actively engaged in promoting Computational Sciences via online Workshops/Hands-on-Training in Academic Institutions and Research Industries. We are proud to say that we are the first to introduce Hands-on-Training (Online and Onsite) on Quantum Chemical calculation via Density Functional Theory Approach.

We are very proud to announce that in a short span of 2 years, we have trained **8000+** Graduate students, Research Scholars, Professors & Industry Experts from 35 countries including the India, US, UK, Saudi Arabia, Mexico, Brazil, Malaysia, Kuwait, Germany, Peru, South Korea, Finland, Turkey, Iraq, Australia, Philippines, Spain, Jordan, Chile, Taiwan, South Africa, Pakistan, Nepal, Bangladesh, Nigeria, Morocco, Egypt, Sri Lanka and Algeria, Singapore, Columbia, Sweden, Botswana, Belgium, Canada and rated 4.78/5.00 by 700+ International and National participants of our previous workshops. The Centre previously had 5 invited lectures:

1. **Dr. Snehasis Daschakraborty,** Asst. Prof. (IIT Patna):[https://www.youtube.com/watch?v=CaZl0iFJU-I]
2. **Prof. T. P. Radhakrishnan,** Prof. (Hyderabad University):[https://www.youtube.com/watch?v=5IWNLsntgSU]
3. **Dr. V. Ramanathan,** Asst. Prof. (IIT BHU): [https://www.youtube.com/watch?v=erKb3y71VN8]
4. **Prof. Kalidas Sen,** Prof. (Emeritus) (Hyderabad University):[https://www.youtube.com/watch?v=jkz_Hb99vEg]
5. **Dr. Ranganathan Subramanian,** Associate Professor (IIT Patna).

Prof. T. P. Radhakrishnan
Professor [University of Hyderabad]
H-Index = 38, Citations = 5046
FNASc, FASc, FNA, Ph. D., Princeton University
Postdoctoral Research, University of Texas at El Paso

DR. SNEHASIS DASCHAKRABORTY
Assistant Professor [IIT Patna]
H-Index = 15, Citations = 702
Postdoctoral Research, University of Colorado

DR. RANGANATHAN SUBRAMANIAN
Associate Professor, IIT Patna
H-Index = 7, Citations = 550
Ph.D, Wesleyan University

PROF. KALIDAS SEN
Professor (Emeritus), Hyderabad University
H-Index = 42, Citations = 6024
F.A.Sc., F.N.A.

DR. V. RAMANATHAN
Assistant Professor [IIT BHU]
H-Index = 11, Citations = 529
Postdoctoral Research, University of Stuttgart, Germany

Certificate (Copy) to be issued.

1ST ONLINE HANDSON-TRAINING ON
DENSITY FUNCTIONAL THEORY OF ADVANCED MATERIAL
(USING QUANTUM ESPRESSO PACKAG

Centre for Advanced Computational Research, New Delhi, India

(Registered under Ministry of SME, Government of India for Research and Experimental Development on Natural Sciences and Engi neering)
(ISO 9001:2015 Certification for Hands-on-Training on Computational Science including DFT calculation of Materials, Molecular Docking and Dynam ics)
Website: https://cacrdelhi.com, Email: admin@trainingcacrdelhi.com

Certificate of FDP Completion

This is to certify that

Sudhanshu Mallick, Professor, India

has actively participated in the **1st Faculty Development Program (FDP) on Density Functional Theory Modelling of Advanced Materials (DFT-Advanced)** organized by the Centre for Advanced Computational Research, Delhi from **25th Feb. – 6th Mar. 2025** via Online Mode. FDP had 10 Interactive Hands-on-Training Sessions by **DR. NIKHIL AGGARWAL** using **Quantum Espresso, Burai** and **Vesta** Software Packages.

Dr. Nikhil Aggarwal
Head of the Department & Convener

ISO Accreditation Body: United Ackreditering Services Limited, United Kingdom
Certificate No.: 2025/DFT-M/F/1/1

1ST ONLINE HANDSON-TRAINING ON
DENSITY FUNCTIONAL THEORY OF ADVANCED MATERIAL
(USING QUANTUM ESPRESSO PACKAG

Centre for Advanced Computational Research, New Delhi, India

(Registered under Ministry of SME, Government of India for Research and Experimental Development on Natural Sciences and Engi neering)
(ISO 9001:2015 Certification for Hands-on-Training on Computational Science including DFT calculation of Materials, Molecular Docking and Dynam ics)
Website: https://cacrdelhi.com, Email: admin@trainingcacrdelhi.com

Certificate of Participation

This is to certify that

Prakash Barfa, Research Scholar, Devi Ahilya Vishwavidyalaya, Indore, Madhya Pradesh, India

has actively participated in the **1st Hands-on-Training Program on Density Functional Theory Modelling of Advanced Materials (DFT-Advanced)** organized by the Centre for Advanced Computational Research, Delhi from **25th Feb. – 6th Mar. 2025** via Online Mode. The training program had 10 Interactive Sessions by **DR. NIKHIL AGGARWAL** using **Quantum Espresso, Burai and Vesta** Software Packages.

Dr. Nikhil Aggarwal
Head of the Department & Convener

ISO Accreditation Body: United Ackreditering Services Limited, United Kingdom
Certificate No.: 2025/DFT-M/W/1/X