1ST ONLINE TRAINING ON

DENSITY FUNCTIONAL THEORY MODELLING AT MOLECULAR LEVEL USING GAUSSIAN (DFT-G)

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@cacr.co.in

Date: 10th February – 16th February 2026

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]

(Participants must have preinstalled Gaussview and Gaussian Software Applications*)

***Participants can check the Supercomputing Resource at their respective Institution (Links on Last Page).**

1. About FDP/Workshop:

We are glad to announce the next **7-Days Online Training FDP/Workshop program on DFT Modelling at Molecular Level using Gaussian [DFT-G]: Spectral (IR, UV, NMR, Raman and Emission Characteristics), Intermolecular Interactions, Chemical Reactions, Charge Transfer Studies.**

- 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 for details

https://www.cacrdelhi.com/dft-molecularlevel

or

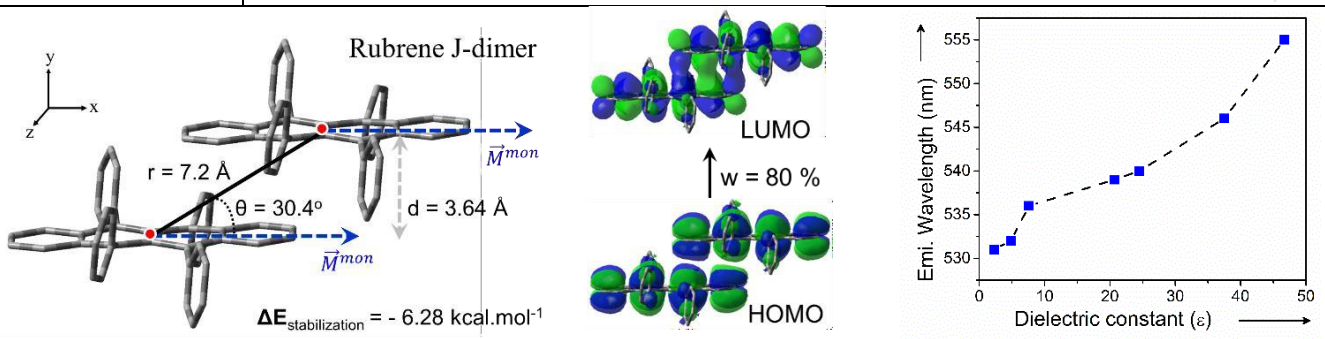
https://www.cacrdelhi.com/event-details/online-training-on-dft-modelling-at-molecular-level-using-gaussian-dft-g

Note: Those registering for the Training are requested to also join WhatsApp Group for quick updates.

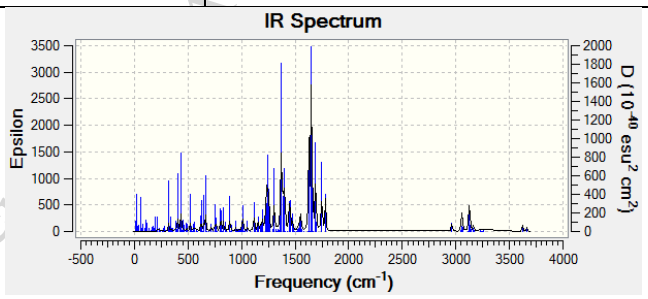
Join our WhatsApp Group

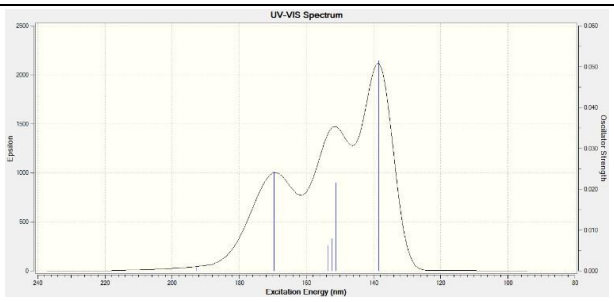
3. Detailed Day wise Schedule

10th February 2026 **Day 1**	**Session 1: Fundamentals** Introduction to Computational Science: Quantum Mechanical vs. Molecular Mechanical Calculations, Density Functional Theory (DFT), Molecular size vs. accuracy vs. Time factor, Molecular Structure Building, Pre-optimization
11th February 2026 **Day 2**	**Session 2: Molecular Structural Optimization** Basis Sets and Functional, Geometry/Structure Optimization, Solvent effect: Implicit model vs. Explicit mode, Solvent Mixtures, Energy Convergence



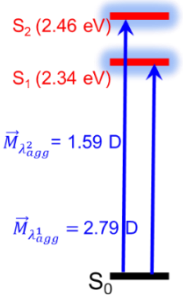
12th February 2026 **Day 3**	**Session 3: Frequency (Infrared Spectrum Computation)** Predict Stability, Dipole Moment Vector, Solubility, Vibrational frequencies (IR Spectrum), Visualization of Vibrational Modes:Stretching vs. Bending, Asymmetric vs. Symmetric Stretching, Negative Frequencies Frequency Shift on: Intermolecular interaction, Adsorption of molecule on surface, Metal Complexation
13th February 2026 **Day 4**	**Session 4: UV-Vis and Raman Spectra Computation** Raman Spectrum Calculation UV spectra, TD-DFT calculations, Singlet vs. triplet excited states, allowed vs forbidden transitions, multimolecular orbital transition, energy level diagram, Photovoltaic activity, Molecular orbital analysis HOMOs vs. LUMOs, Orbital Contribution

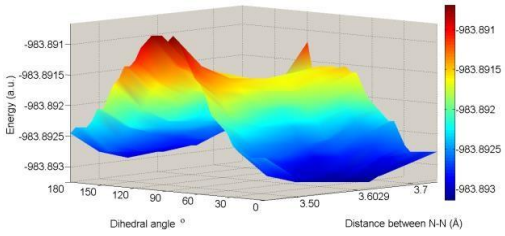


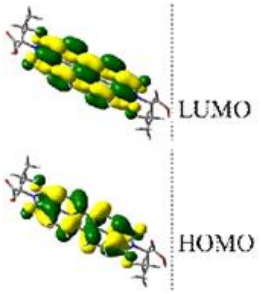


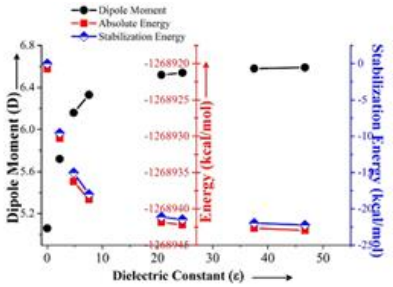
14th February 2026 **Day 5**	**Session 5: NMR Spectrum Computation** Hardness, Softness, Chemical Potential, Electronegativity and Electron Affinity, NMR Spectrum Calculation (C^{13}, H^1), Chemical Shift.

15th February 2026 **Day 6**	**Session 6: Adsorption (Intermolecular Interactions)** Adsorption: Intermolecular interactions between Adsorbate and Adsorbent, Single-Point Energy, Potential Energy Surface Diagrams, Optimized Binding Distances

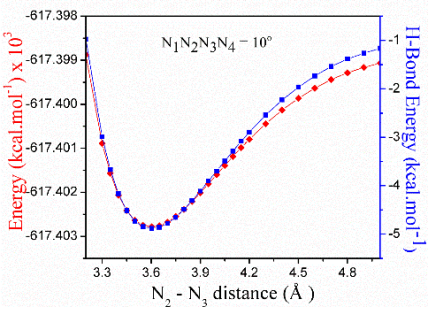


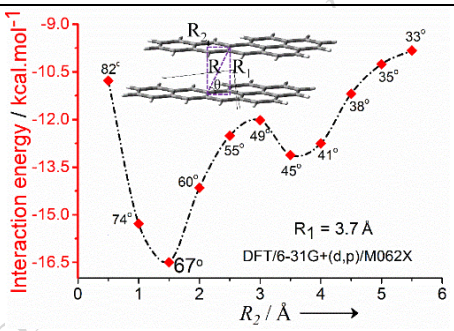






16th February 2026 **Day 7**	**Session 7: Chemical Reaction and Charge Transfer** Reaction Mechanism, Enthalpy of reactions: Exothermic vs. Endothermic, Transition State Structures, Activation Energy, Intermediates, Charge Transfer





4. Salient Features

- ✓ **Participants must have preinstalled Gaussview and Gaussian Software Applications: The Centre will not share the Software**
- ✓ **Eligibility:** Candidate must have knowledge of undergraduate level science.
- ✓ Sessions will be taken via online mode, Lecture Mode: English
- ✓ e-certificates will be provided to all registered participants
- ✓ Training will be provided on Windows Operating system
- ✓ Programming and coding knowledge is **not required** for above Training.

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/Industry Expert/Scientist	Rs. 2,500
Non-Indian Participants	Rs. 4100 or USD 48

Certificate (Copy) to be issued

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Certificate of FDP Completion

This is to certify that **Dr. Raj Kaushal, Assistant Professor, National Institute of Technology (NIT) Hamirpur, Himachal Pradesh** has actively participated in the **1st Faculty Development Program (FDP) on Density Functional Theory Modelling at Molecular Level using Gaussian: Spectral (IR, UV, NMR, Raman and Emission Characteristics), Intermolecular Interactions, Chemical Reactions, Charge Transfer Studies (DFT-G)** organized by the Centre for Advanced Computational Research, Delhi from **10th February – 16th February 2026** via Online Mode. FDP included 7 Interactive Sessions on both Ground and Excited States computations.

Dr. Nikhil Aggarwal
Head of the Department & Convener

ISO Accreditation Body: United Ackreditering Services Limited, United Kingdom
Certificate No.: 2026/DFT-G/F/1/x

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Centre for Advanced Computational Research, New Delhi, India

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Website: https://cacrdelhi.com, Email: admin@cacr.co.in

Certificate of Participation

This is to certify that **Arnab Mandal, Research Scholar, IISER BHOPAL, MADHYA PRADESH, INDIA** has actively participated in the **1st Hands-on Training on Density Functional Theory Modelling at Molecular Level using Gaussian: Spectral (IR, UV, NMR, Raman and Emission Characteristics), Intermolecular Interactions, Chemical Reactions, Charge Transfer Studies (DFT-G)** organized by the Centre for Advanced Computational Research, Delhi from **10th February – 16th February 2026** via Online Mode. FDP included 7 Interactive Sessions on both Ground and Excited States computations.

Dr. Nikhil Aggarwal
Head of the Department & Convener

ISO Accreditation Body: United Ackreditering Services Limited, United Kingdom
Certificate No.: 2026/DFT-G/W/1/x

6. About Us

Global Impact Through Online Training of Innovative Minds from 70+ Countries

Awarded with ISO 9001:2015 Certification: Accredited by UASL, UK

4 Keynote Lectures on Recent Advances in Computational Chemistry by Eminent Scientists

4.75/5.00 Ratings with excellent reviews from 700+ Participants

Trained 1206 Faculties, 120 Postdoctorates, 2696 Research Scholars, 685 Students

Welcome to the Centre for Advanced Computational Research (CACR), based in New Delhi, India, was founded in April 2021, is a distinguished institution that is at the forefront of advancing knowledge and expertise in the realm of computational science. Our expertise encompasses analytical chemistry, the synthesis of organic and inorganic chemicals, pharmaceuticals, and bioinformatics. Endorsed by the Ministry of SME, Government of India, we are committed to promoting research and experimental development within the domains of natural sciences and engineering. Furthermore, our institution holds the ISO 9001:2015 Certification, reflecting our dedication to delivering exceptional hands-on training in computational science, including DFT calculations, molecular docking, and dynamics. Our research and development initiatives concentrate on extensive spectroscopic investigations of novel materials through advanced chemistry methodologies. We seek to examine their applications across a wide range, including organic light-emitting diodes (OLEDs), photovoltaics, catalysis polymer design, and energy-based materials. Furthermore, our efforts encompass optoelectronic devices, non-linear optical activity, energy transfer mechanisms, and bioinformatics. Through these cutting-edge approaches, we make significant contributions to the advancement of technology and materials science. The Centre has installed two advanced workstations to further enhance our research activities. This infrastructure investment underscores our commitment to fostering innovative research and development.

About Speaker: Dr. Nikhil Aggarwal [Acad. Head, CACR; Ph.D. (IIT Madras), M.Sc. & B.Sc. (DU)

Currently, our organization is under the leadership of Dr. Nikhil Aggarwal, who brings a wealth of knowledge and experience in the computational investigation of molecules, utilizing various Density Functional Theory (DFT) approaches. Dr. Aggarwal earned his Ph.D. in Physical Chemistry from the prestigious Department of Chemistry at IIT Madras in 2017, and he also holds both an M.Sc. and B.Sc. from the University of Delhi. With an impressive portfolio that includes five publications in highly respected international journals, such as those published by the American Chemical Society and Wiley, as well as a book published by Lambert Publishing House in Germany, Dr. Aggarwal has made significant contributions to the field. Furthermore, he was an active participant in the International Conference on Modern Computational Methodologies and Challenges held at the University of Washington, USA, in 2016. The organization supported by 18 project students from prestigious research institutions in India and abroad, including IISC Bangalore, IITs, NITs, and CSIR Labs.

About Hands-on Training

We are actively committed to promoting computational science through online workshops and hands-on training in academic institutions and research industries. We take pride in being the first to offer hands-on training, both online and onsite, in quantum chemical calculations using Density Functional Theory (DFT) approaches. Our initiatives aim to equip participants with practical skills and knowledge in critical areas of research. By fostering collaboration and education, we strive to advance the field of computational science. We are proud to announce that in just 4 years, we have successfully trained over 5,000 graduate students, research scholars, professors, and industry experts from 70 countries, including the US, UK, Saudi Arabia, Mexico, Brazil, Malaysia, Kuwait, Germany, Peru, South Korea, India, 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. Our efforts have garnered a rating of 4.76 out of 5.00 from more than 700 international and national participants in our previous workshops. This achievement reflects our commitment to providing high-quality training and education in computational chemistry. We look forward to continuing our mission of empowering individuals across the globe with valuable skills and knowledge.

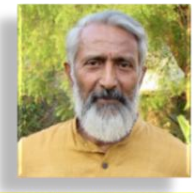
Centre has had the privilege of hosting five invited lectures by renowned computational chemistry researchers from prestigious research institutions. These sessions offered valuable insights and encouraged dynamic discussions on the latest developments in the field. We are dedicated to promoting knowledge exchange and collaboration within the scientific community. The Centre previously had 5 invited lectures:

1. **Dr. Snehasis Daschakraborty,** Assistant Professor, Indian Institute of Technology Patna
2. **Prof. T. P. Radhakrishnan,** Professor, Hyderabad University
3. **Dr. V. Ramanathan,** Assistant Professor, Indian Institute of Technology BHU
4. **Prof. Kalidas Sen,** Professor (Emeritus), Hyderabad University
5. **Dr. Ranganathan Subramanian,** Associate Professor, Indian Institute of Technology 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

Thank you to the Top 50 Faculty for attending our Training!

Your commitment is Inspiring

1. Dr. Susantha Ganegamage, Assistant Professor at **Lamar University, Texas**, United States of America (USA) **DFT-G**
2. Dr. Binod R Giri, Senior Research Scientist at **King Abdullah University of Science and Technology** (KAUST), Saudi Arabia **DFT-G**
3. Dr. Shaza Massarani, Professor (Full) at **King Saud University** (KSU), Saudi Arabia **DFT-G**
4. Dr. Aziz Unnisa, Associate Professor at the **University of Hail** (UOH), Saudi Arabia **DFT-G**
5. Dr. Abdel-Baset H. Mekky, Professor (Associate), **Qassim University** (QU), Saudi Arabia **DFT-G**
6. Dr. Hela Ferjani, Professor (Associate), **Imam Mohammad ibn Saud Islamic University** (IMSU), Saudi Arabia **DFT-G**
7. Dr. Felipe Cordova LozanoFundación, Professor, **Universidad de las Américas**-Puebla (UAP), Mexico **DFT-G**
8. Dr. Murali Venkata Basavanga Unnamatla, Fulltime Professor, **Universidad Autónoma del Estado de México** - Inicio (UEE), Mexico **DFT-G**
9. Dr. Jose Manuel Bravo-Arredondo, Professor (Associate), **Autonomous University of Tlaxcala** (UOT), Mexico **DFT-G**
10. Dr. Syed Shaheen Shah, Assistant Professor, **Kyoto University** (KU), Japan **DFT-G**
11. Dr.Elhassane Mohamed Abdssalam Anouar, Associate Professor, **Prince Sattam bin Abdulaziz University** (PSAU), Saudi Arabia **DFT-G**
12. Prof. (Dr.) Amartya Sengupta, Professor, **Indian Institute of Technology** (IIT) **Delhi**, Delhi, India **DFT-G**
13. Prof. (Dr.) Arindam Sarkar, Professor, **Indian Institute of Technology** (IIT) **Bombay**, Maharashtra, India **RRD**
14. Prof. (Dr.) Chandramohan Palogi, Professor, **Homi Bhabha National Institute**, Maharashtra, India **RRD**
15. Prof. (Dr.) Manikandan P, Professor, **Indira Gandhi Centre for Atomic Reserach** (IGCAR), Kalpakkam, Tamil Nadu, India **RRD**
16. Prof. (Dr.) Rajesh Prasad, Professor, **Indian Institute of Technology** (IIT) **Delhi**, Delhi, India **RRD**
17. Prof. (Dr.) Santu Dey, Professor, **Variable Energy Cyclotron Centre**, India **DFT-M**
18. Prof. (Dr.) Subrato Bhattacharya, Professor, **Banaras Hindu University**, Uttar Pradesh, India **DFT-G**
19. Prof. (Dr.) Vinod Kumar Kannaujiya, Professor, **Banaras Hindu University** (BHU), Uttar Pradesh, India **DFT-G**
20. Prof. (Dr.) Krishna Kumar Singh, Professor, **Birla Institute of Technology and Science** (BITS) Pilani, Dubai, United Arab Emirates **DFT-M**
21. Prof. (Dr.) Prashant Kharkar, Professor, **Institute of Chemical Technology** (ICT), Mumbai, Maharashtra, India **CADD**
22. Prof. (Dr.) Bivas Dam, Professor, **Jadavpur University** (JU), West Bengal, India **RRD**
23. Prof. (Dr.) Ozair Alam, Professor, **Jamia Hamdard University** (JHU), New Delhi, India **CADD**
24. Prof. (Dr.) Satyajit Banerjee, Professor, **Indian Institute of Technology** (IIT) **Kanpur**, India **DFT-M**
25. Prof. (Dr.) Parnika Das, Professor, **Homi Bhabha National Institute** (HBNI), India **DFT-M**
26. Dr. Sandeep Pokharia, Professor, **Banaras Hindu University** (BHU), Uttar Pradesh, India **DFT-M**

27. Dr. Surendra Singh, Associate Professor, **Homi Bhabha National Institute** (HBNI), Maharashtra, India **DFT-M**
28. Dr. Rajeev Kumar, Associate Professor, **Homi Bhabha National Institute** (HBNI), Maharashtra, India **DFT-M**
29. Dr. R C Das, Associate Professor, **Homi Bhabha National Institute** (HBNI), Maharashtra, India **DFT-M, DFT-M_A, RRD**
30. Dr. Ajish Kumar K S, Assistant Professor, **Bhabha Atomic Research Centre** (BARC), Maharashtra, India **DFT-M**
31. Dr. Abhijeet L. Sangle, Assistant Professor, **Indian Institute of Technology** (IIT) **Bombay**, Maharashtra, India **RRD, DFT-M**
32. Dr. Apurav Guleria, Assistant Professor, **Homi Bhabha National Institute** (HBNI), Maharashtra, India **DFT-M, RRD**
33. Dr. Bani Mahanti, Assistant Professor, **Banaras Hindu University** (BHU), Uttar Pradesh, India **DFT-G**
34. Dr. D N V V Konda Lutukurthi, Assistant Professor, **Indian Institute of Technology** (IIT-ISM) **Dhanbad**, Jharkhand, India **DFT-G, DFT-M**
35. Dr. Debasish Manna, Assistant Professor, **Indian Institutes of Science Education and Research** (IISER) **Bhopal**, Madhya Pradesh, India **DFT-G**
36. Dr. Divya Kushwaha, Assistant Professor, **Banaras Hindu University**, Uttar Pradesh, India **DFT-G**
37. Dr. Kodanda Ram Mangipudi, Assistant Professor, **Indian Institute of Technology** (IIT) **Bhubaneswar**, Odisha, India **RRD**
38. Dr. R Lalneihpuii, Assistant Professor, **Banaras Hindu University**, Uttar Pradesh, India **DFT-G**
39. Dr. Rahul Sharma, Assistant Professor, **Indian Institutes of Science Education and Research** (IISER) **Berhampur**, Odisha, India **DFT-M**
40. Dr. Sandeep Patel, Assistant Professor, **Banaras Hindu University** (BHU), Uttar Pradesh, India **DFT-G**
41. Dr. Santanu Mandal, Assistant Professor, **Indian Institute of Technology** (IIT) **Bhubaneswar**, Odisha, India **DFT-M, DFT-M_A**
42. Dr. Selvakumar Jayaprakasam, Assistant Professor, **Homi Bhabha National Institute** (HBNI), Tamil Nadu, India **DFT-M**
43. Dr. Sonal Shrivastava, Assistant Professor, **Indian Institute of Technology** (IIT) **Patna**, Bihar, India **RRD**
44. Dr. Sree Rama Murthy Anupindi, Assistant Professor, **Homi Bhabha National Institute** (HBNI), Maharashtra, India **DFT-G**
45. Dr. Subhas Samanta, Assistant Professor, **Indian Institute of Technology** (IIT) **Jammu**, Jammu and Kashmir **DFT-G**
46. Dr. Sumit Kamal, Assistant Professor, **Indian Institute of Technology** (IIT) **Jodhpur**, Rajasthan, India **DFT-G, DFT-M**
47. Dr. Supriyo Ghosh, Assistant Professor, **Indian Institute of Technology** (IIT) **Roorkee**, Uttarakhand, India **DFT-M**
48. Dr. Sushil Kumar, Assistant Professor, **Homi Bhabha National Institute**, Maharashtra, India **DFT-G**
49. Dr. Veeramani Chidambaranathan, Assistant Professor, **Indian Institute of Technology** (IIT) **Roorkee**, India **DFT-M**
50. Dr. Venkatadivakar Botcha, Assistant Professor, BioSense Institute, **University of Novi Sad**, Novi Sad, Serbia **DFT-M**

Ramesh Das

I, R C Das am a **faculty at Homi Bhabha National Institute**. I attended a 7 days online session on Materials Modelling at DFT level using Quantum Espresso hosted by Dr. Nikhil Aggarwal at Centre for Advanced Computational Studies from 4 Feb. - 10 Feb. 2024.

This short course has helped me to understand the basics in a very practical manner. I highly appreciate the guidance of Prof. (Dr.) Nikhil Aggarwal.

Apurav Guleria

I (Dr. Apurav Guleria) am a **faculty at Homi Bhabha National Institute** (HBNI), Anushakti Nagar, Mumbai. I attended a 7 days online session on Materials Modelling at DFT level using Quantum Espresso hosted by Dr. Nikhil Aggarwal at Centre for Advanced Computational Studies from 12 - 18 Oct 2023. It was a well-organized work-shop. Important aspects of this work-shop were suitable timings (9-10 PM online) and recordings provided by Dr. Nikhil. The course prepared/and taught was very much helpful for new beginners like me in computational field. I would definitely like to attend such work-shops in the future also, especially on the use of Gaussian software and other computational tools.
Thanks & Regards

Rajib Ghosh Chaudhuri

I, Rajib Ghosh Chaudhuri, am a **faculty member at the National Institute of Technology Durgapur**. I attended a 10-day online Hands-on-Training program on DFT Modelling of Advanced Materials using Quantum Espresso, hosted by Dr. Nikhil Aggarwal at the Centre for Advanced Computational Research from 8 Apr. - 17 Apr. 2025. It is a very nice interactive hands-on training session. Dr. Nikhil is very energetic and knowledgeable person. I will recommend that all interested beginners try for this session.

Dr. Ganesh Lal

I Dr. Ganesh Lal am a **faculty at Hansraj College University of Delhi**. I attended a 7-Days online session on Materials Modelling at DFT level using Quantum Espresso hosted by Dr. Nikhil Aggarwal at the Centre for Advanced Computational Research from 28 Apr. - 4 May 2024. I was registered for earlier session that was about to 9 April, but the session was postponed due less number registered candidates so due to my engagement in other work I could not attend all session but the session I attended was very helpful and informative. I am very impressed with Dr. Nikhil sir how clearly; he explains everything and take all queries of from the candidates. Thank you Sir

Dr. Prikshit Gautam

I, Dr. Prikshit am a **faculty at Kirori Mal College University of Delhi**. I attended 7 days online session on Materials Modelling at DFT level using Quantum Espresso hosted by Dr. Nikhil Aggarwal at Centre for Advanced Computational Studies from 26 Nov - 2 Dec. 2023. I thank Dr. Nikhil, who made data handling using Quantum Espresso very easy to understand and its application to various systems looks very simple now. I am very excited to apply this on my system on which i am working on l

Thank u once again

Arpita Vajpayee

Hello. I Dr Arpita Vajpayee am a **faculty at Dyal Singh College University of Delhi**. I attended a 7-days online session on Molecular Modelling at DFT level hosted by Dr. Nikhil Aggarwal at Centre for Advanced Computational Research from 14 May - 20 May 2024. I believe that the transaction pedagogy has been very good. Knowledge content was also of utmost relevance and in consonance with the objectives and goals of the program. However, a continuity of lectures could help to cover all the topics in complete respect in stipulated time.

Bello Kehinde

I Abdulraheem Bello am a research graduate at _____SAUDI ARABIA___/(KFUPM). I attended a 7-Days online Hands-on-Training program on Molecular Modelling at DFT level hosted by Dr. Nikhil Aggarwal at the Centre for Advanced Computational Research from 30 Apr. - 6 May 2024.

The training session was very helpful in understanding the key and important areas of simulation by Gaussian and answers some hidden information in research articles as well as how to respond to reviewers' comment. It was indeed what the time and the money.

Sunny Choudhary

I, Sunny Choudhary, am a research scholar at University of Puerto Rico, USA. I attended online session on Materials Modelling at DFT level using Quantum Espresso hosted by Dr. Nikhil Aggarwal at Centre for Advanced Computational Studies from 02 - 14 Nov 2023. This session was very helpful to understand the computational significance in the research work. Thanks to Dr. Nikhil for giving hands on training.

Divakar Botcha

I, Dr. Divakar Botcha, am a research faculty at the BioSens Institution at the University of Novi Sad, Serbia. Dr. Nikhil Aggarwal hosted an online session for Materials Modelling at DFT level using Quantum Espresso that I attended for a total of 7 days. It was a wonderful program and thank you very much.

Trupti Mohanty

I am Trupti, currently pursuing my graduate studies at the University of Utah. I recently participated in a week-long online workshop on Materials Modelling at the DFT level using Quantum Espresso, which was conducted by Dr. Nikhil Aggarwal. This experience was truly enriching, as it provided me with a deep understanding of software applications and their diverse practical uses. I am eager to explore more training programs in the realm of computational chemistry in the future.

Durga Prasad Khatua

I am Durga Prasad Khatua, postdoctoral scholar at UCLA. I attended a 7 days online session on Materials Modelling at DFT level using Quantum Espresso hosted by Dr. Nikhil Aggarwal at Centre for Advanced Computational Studies from 12 - 18 Oct 2023.
As a research scholar attending the recent lecture on DFT by Nikhil sir, I must say that it was a truly enlightening experience which left a lasting experience on me. Some key points of the lecture series are

1) clarity 2) response to each and every doubt 3) inspiration. Thank you so much Nikhil sir for the DFT lecture series and for sharing your experience.

Shamila Gopalakrishnan

I m a just fresh graduate from USJP, currently in Sri Lanka. doing synthesis and characterization of novel compounds. But I have a long desire to learn computational chemistry to enhance myself and handle molecules workable. His workshop was impressive...I

attended molecular docking and basic MSD. Worth it .... I really enjoyed the session and even his patience in teaching, crystal clear explanations and interest to answer every question in the class asked by students helped me to gain knowledge. Thank u sir.

Sayed Newaj Chowdhury Nishan

I, Sayed Newaj Chowdhury Nishan, am an undergraduate student at Gopalganj Science and Technology University, Bangladesh. I attended a 10-day online session on DFT Modelling of Advanced Materials using Quantum Espresso hosted by Dr. Nikhil Aggarwal at the Centre for Advanced Computational Research from 4 to 13 Mar 2025. During the session, I gained hands-on experience with Quantum Espresso, performing DFT calculations for advanced materials. I also deepened my understanding of electronic structure analysis and material property predictions.

AARTI RAJPUT

I am Aarti Rajput a research scholar at IIT BHILAI. I attended a 7-Days online Hands-on-Training program on DFT Modelling at Molecular Level hosted by Dr. Nikhil Aggarwal at the Centre for Advanced Computational Research from 15 Apr. - 21 Apr. 2025. The modelling is based on the basic understanding of the concept and the motivation for the advanced level modelling. I really thankful for the sessions given by them.

Yeshvanth S

I Yeshvanth S am a research scholar at Indian Institute of Technology Dharwad. I attended a 7-Days online Hands-on-Training program on DFT Modelling at Molecular Level hosted by Dr. Nikhil Aggarwal at the Centre for Advanced Computational Research from 17 Apr. - 23 Apr. 2025. The workshop was helpful and I learned to setup my DFT calculations for my own research molecules.

Abhishek Raman

I am Abhishek Raman, a research scholar at IIT Roorkee. I attended a 7-Days online Hands-on-Training program on DFT Modelling at Molecular Level hosted by Dr. Nikhil Aggarwal at the Centre for Advanced Computational Research from 18 Mar - 24 Mar 2025. I learned how to use gauss view and gaussian and also various methods of DFT. This training program is really very helpful and it will be definitely useful in my research work in the coming days.

Sandeep Gupta

I Sandeep Gupta, am a research scholar at Indian Institute of Technology, Roorkee. I attended a 7-Days online Hands-on-Training program on Molecular Modelling at DFT level hosted by Dr. Nikhil Aggarwal at the Centre for Advanced Computational Research from 30 Apr. - 6 May 2024. It was quite helpful for my field of interest. I heartly thanks to Dr. Nikhil Aggarwal sir. His way of explaining the topics cleared my doubts. Thanks!

Naveen Kumar

I Naveen Kumar Arkoti, a research scholar at Indian Institute of Technology Roorkee. I attended a 7 days online session on Materials Modelling at DFT level using Quantum Espresso hosted by Dr. Nikhil Aggarwal at Centre for Advanced Computational Studies from 14 Sep - 20 Sep 2023. This training helped me to understand the DFT concepts, DOS and bandgap calculations and plotting for simple and heterostructures. I thank you for providing such a nice and informative training.

Dr. Juhi Dutta

I am Dr. Juhi Dutta, a postdoctoral research scholar at Indian Institute of Technology Guwahati. I attended a 7 days online session on Materials Modelling at DFT level using Quantum Espresso hosted by Dr. Nikhil Aggarwal at Centre for Advanced Computational Studies from 4 Feb. - 10 Feb. 2024. I am glad that I have taken the hand on training program on DFT-M. I had a very little idea about the Softwares used in computational study of the materials i.e., in solid state chemistry. The best thing was that we could get the recordings if we have missed any session or a part of it. Starting from the installation of the software to running the calculations, everything has been covered within this 7-day workshop. I am grateful to Dr. Nikhil Aggarwal for initiating such kind of insightful and enlightening hand-on-training online workshop. Thank you.

Sirsendu Ghosal

I, Sirsendu Ghosal am a research scholar at IIT Guwahati. I attended a 7-days online session on molecular modelling at DFT level hosted by Dr. Nikhil Aggarwal at Centre for Advanced Computational Research from 14th may - 20th may. I would like to convey my regards to Sir for taking this kind initiative for students like us. All of the sessions were very enjoyable and the basics of the topics were explained in detail. Moreover, the queries regarding our own research problems were also elaborated quite nicely. Thanks to these sessions, I am now able to perform my own calculations independently. I look forward to more such sessions and discussions in the upcoming days.

Asmita Sikdar

I Asmita, a researcher at IIT G. I attended a 7-Days online hands-on training program on Molecular Modelling at DFT level hosted by Dr. Nikhil Aggarwal at the Centre for Advanced Computational Research from April 30 to May 2024. The workshop was really helpful for experimental researchers who have little knowledge regarding DFT. I believe this will be helpful for my future research career.

Shamim Shah

My name is Shamim Hossain Shah, a PhD student at Centre for Nanotechnology, IITG, India. I joined the 6th CCW after one of my friends informed me. Before that I was looking for tutorials on YouTube but that didn't help me a lot. Everything was going over my head. In the introductory class I was convinced that this is gonna be a great journey. Although I was a beginner, I have learned a lot of things as the workshop kept on progressing. I have gained knowledge about how to use Gaussian effectively before we reached at the final day of the workshop.
I would like to recommend everyone who is planning to use Gaussian to enhance their manuscript. The workshop is very interactive so any and every doubt of yours will be answered. Finally, I would say that this workshop will establish the basic foundation in working with Gaussian for beginners like me. I would like to quote Dr. Nikhil - " There's a whole lot of information embedded in the Gaussian results which you can put in your manuscripts".

Md Abdus Salam Shaik

I, Md Abdus Salam Shaik, student from IIT Kharagpur. I have attended 7-days online workshop on Molecular modelling at DFT level organised by Dr. Nikhil Aggarwal at Centre for Advance Computational Research from 14-23 May.
I am really grateful to Dr. Nikhil Sir to organised such a useful and insightful session for us. Every nitty-gritty about the course have been perfectly delivered within the given time. I am really hopeful to participate this type of session in future.

Manisha Shaw

I Manisha Shaw am a research scholar at the Indian Institute of Technology Kharagpur (IIT KGP). I attended a 7-day online session on Materials Modelling at the DFT level using Quantum Espresso hosted by Dr. Nikhil Aggarwal at the Centre for

Advanced Computational Studies from 14 Sep - 20 Sep 2023. Here, I learned many major and minor technicalities required for running a job in QE, without which I was facing a lot of issues. Although many videos are already there on YouTube, they don't speak much about the technicalities. So, this 7-day session was really helpful for me.

RABEYA BASORI

I (Rabaya Basori) am a research scientist at IIT Kharagpur. I attended a 7 days online session on Materials Modelling at DFT level using Quantum Espresso hosted by Dr. Nikhil Aggarwal at Centre for Advanced Computational Studies from 4 Mar. - 10 Mar. 2024.I am an experimentalist. This is the first computational/theoretical workshop/training program I have attended and appreciate it very much. This makes me capable my experimental results to explore or rather verify with theoretical approach too.
DFT is widely used in theoretical physis as well as material science. We have got just a glimpse of it. We need more lengthy training program to fully utilize the software.

Besides, we are very much thankful to Dr. Nikhil Aggarwal, our coordinator of the training program. Dr. Aggarwal has very good teaching skills, patience and strong communication skills with all the participants.

In future, if Centre for Advanced Computational Research arrange such program in advanced level that will be really helpful for us. Thank you Dr, Aggarwal. Thanks to the Centre for Advanced Computational Research for arranging nice program.

Bidipta Dam

I, Bidipta Dam, am a research scholar at IIT Kharagpur. I attended a 7 days online session on Materials Modelling at DFT level using Quantum Espresso hosted by Dr. Nikhil Aggarwal at Centre for Advanced Computational Studies from 26 Nov - 2 Dec. 2023. The course was very detailed and very helpful for research purposes. Detailed calculation regarding DFT modelling was taught. Hope more such courses will be conducted in the future. These are very beneficial for research scholars.

Suprabha Charjren Lakra

I Suprabha Charjren Lakra am a post graduate at Indian Institute of Technology Kharagpur. I attended a 7 days online session on Materials Modelling at DFT level using Quantum Espresso hosted by Dr. Nikhil Aggarwal at Centre for Advanced Computational Studies from 14 Sep - 20 Sep 2023. I have hands-on experience in a training program focused on Density Functional Theory (DFT) Modelling of materials: Nanoparticles, Thin Films, Unit Cells (DFT-M), using Free License Software Tools: Quantum Espresso. During this program, I gained expertise in using DFT software tools, performing electronic structure calculations, and simulating material properties, which has enriched my understanding of materials science and computational chemistry.

Koninika

I, Koninika a research scholar/faculty at IIT Bombay. I attended a 7-day online hands-on training program on DFT Modelling at the Molecular Level hosted by Dr. Nikhil Aggarwal at the Centre for Advanced Computational Research from 15 Apr. - 21 Apr. 2025. The program provided valuable practical exposure to density functional theory (DFT) techniques and their applications in molecular-level simulations. The sessions were well-structured, combining theoretical concepts with hands-on exercises using real computational tools. This training significantly enhanced my understanding of DFT-based Modelling and its relevance to ongoing research in materials and molecular science.

Sutonu Sadhukhan

I, Sutonu Swapan Sadhukhan, am a PhD Student @ IIT Bombay. I attended a 7 days online session on: Materials Modelling at DFT-level using: Quantum Espresso hosted by: Dr. Nikhil Aggarwal @ Centre for Advanced Computational Studies from: Nov. 26 - Dec. 2, 2023. It was really a great experience. All of the recordings were shared with the participants. Most of the Software-Workshops I've attended before ran in a hustled mode &, were difficult to catch-up. But this one was very gentle, easy to catch-up. Care was taken at individual-level if stuck during: installations &/or, solving problems.

Nikhil Borse

I Nikhil Borse am a research scholar at Indian Institute of Technology Bombay. I attended a 7 days online session on Materials Modelling at DFT level using Quantum Espresso hosted by Dr. Nikhil Aggarwal at Centre for Advanced Computational Studies from 14 Sep - 20 Sep 2023. The session is very useful for researcher. I like about this course is all doubts are clear during session. I strongly recommend each research scholar working on Material should attend this course.

Manish Joshi

I, Manish Chandra Joshi, am a research scholar at Indian Institute of Technology Hyderabad. I attended a 7-day online session on Materials Modelling at DFT level using Quantum Espresso hosted by Dr. Nikhil Aggarwal at Centre for Advanced Computational Studies from 14 Sep - 20 Sep 2023. It was a nice little experience on a DFT tool which I initially thought would be difficult to learn. However, Dr. Nikhil made it simple enough for me to learn it without any difficulty. This knowledge will certainly help me in my future research journey. I sincerely thank Nikhil sir for this wonderful experience and wish him all the best for his future endeavours.

Ramesh K

I am Ramesh from IIT HYDERABAD. I have attended 12th CCG Workshop organized by Dr. Nikhil under Professional Training program.

My experience was very good and I really loved the workshop. Dr. Nikhil has intensified knowledge and he is professional, patience and very clear to answer all the queries. I have garnered a very good knowledge in Gaussian now. Thank you very much, Sir!

Sameer Ahmad Khan

I am a research scholar at the Indian Institute of Technology Delhi. I attended a 7-Days online Hands-on-Training program on Molecular Modelling at DFT level hosted by Dr. Nikhil Aggarwal at the Centre for Advanced Computational Research from 30 Apr. - 6 May 2024. It was an enriching experience filled with knowledge. I would recommend this to acamadecian who are interested in molecular simulation.

Sakshi Garg

Respected Sir, I Sakshi Garg a research scholar at Indian Institute of Technology Delhi. I attended a 7 days online session on Materials Modelling at DFT level using Quantum Espresso hosted by Dr. Nikhil Aggarwal at Centre for Advanced Computational Studies from 14 Sep - 20 Sep 2023. I am working on the experimental part of 2D materials. These materials have layer-dependent optical properties which can be easily visualised using DFT. That's why, I wanted to learn DFT. I am very much thankful to Dr. Nikhil Aggarwal Sir for introducing this subject in an easy way. The explanation he gives is very crisp and clear. Looking forward to learn more from him. Thanks again.

Ashish Dhillon

I am Ashish Dhillon from IIT Delhi, India. I attended 7th CCW using gaussian software from Dr Nikhil under professional training program.
My experience is very good. He has managed the workshop the very well and in a sequenced manner and tried to clear the doubts in every aspect.

I hope this series will be going well in future.

Amisha Bansal

I (Amisha Bansal) am a research scholar at IIT Delhi. I attended a 7-day online session on molecular modelling at DFT level hosted by Dr. Nikhil Aggarwal at Centre for Advanced Computational Research from 30 April - 6 May 2024. I have learnt a lot many new in this session. It was a great experience to deal with different molecules and learn how to operate them.

Souradeep Bhattacharya

I Souradeep Bhattacharya am a research scholar/faculty at Indian Institute of Technology, Indian School of Mines, Dhanbad. I attended a 7 days online session on Materials Modelling at DFT level using Quantum Espresso hosted by Dr. Nikhil Aggarwal at Centre for Advanced Computational Studies from 12 - 18 Oct 2023. It was an enlightening session where I got a personalized and even one-to-one learning experience, especially for complex topics. Dr. Aggarwal is an excellent instructor helping all of us personally even after the course timings. I got a headstrong start to learning DFT that would be prove to be a boon in my future endeavours in material research.

Manan Kothari

I am a student at BHU, in final semester of my Graduation in Chemistry and an attending student in 12th Work shop on Computational Chemistry, molecular modelling and origin and endnote training. Earlier I was not sure about getting myself enrolled and now as I am into it as it's not usually considered to be main stream unless you are into research. I would like to say that I am glad I took the right decision of enrolling myself. I have never been exposed to quantum mechanical computation ever and I can say never ever had a vague idea of how transforming it is and I am drawn towards it even more now as I wanted to research in medicinal chemistry and ADCs Gladly, I would keep learning and be motivated and mentored by Respected Dr. Nikhil Aggarwal sir.

Ram Ratan

I have attended a 7-Days online Hands-on-Training program on Molecular Modelling at DFT level hosted by Dr. Nikhil Aggarwal at the Centre for Advanced Computational Research from 30 Apr. - 6 May 2024. It was a helpful and insightful session. In 7-days. I learn a lot of new things. I have also attended Density functional theory Modelling of material. It was a great help for me to begin with. Along with hands-on training, he also explains the important concepts and clears the doubt. I enjoyed learning with him.

Vivekanand Sharma

I am Vivekanand from IIT Kanpur, India. I attended 4th Computational Chemistry Workshop on Gaussian software from Dr. Nikhil under Professional Training program of the AIMs Institute.

My experience was very good.

Liked:
1. Excellent time management

2. Good for beginner (Should have at least heard about DFT. It would be easier to cope up with the training session).
3. Good effort to make people understand about his/her doubt.
4. Providing recorded videos and PPT is a good way to make people learn.

Disliked:
1. Choosing only organic moiety for demonstration while many people have requested about inorganic complexes as a example.
2. Please demonstrate the nanomaterial too.

Finally Kudos to Dr. Nikhil and his team for organizing such a great workshop for those who are novice to computational chemistry. Thanks.

Saurabh Srivastava

I, Saurabh Srivastava, am a research scholar/faculty at Indian Institute of Technology Kanpur. I attended a 7 days online session on Materials Modelling at DFT level using Quantum Espresso hosted by Dr. Nikhil Aggarwal at Centre for Advanced Computational Studies from 14 Sep - 20 Sep 2023. This was a very useful session for me as I am working on hybrid organic inorganic perovskite materials used for photovoltaic applications. I will apply the knowledge acquired in the session for optimizing the perovskite system as well as calculate the bandgap of the material for different stoichiometry of the compound.

Shashikant Gupta

I Shashikant Gupta, am a research scholar at Indian Institute of Technology Kanpur. I attended a 7 days online session on Materials Modelling at DFT level using Quantum Espresso hosted by Dr. Nikhil Aggarwal at Centre for Advanced Computational Studies from 14 Sep - 20 Sep 2023. The workshop was very well conducted by Dr. Aggarwal. The sessions were very interactive. Live projects were conducted and several queries were also resolved during the sessions. After the completion of the workshop, I am excited enough to explore the DFT as a learning tool for polymeric materials and simulating their functional properties.

Thank You

Important e-resources (Supercomputing and Required Software Applications)

Dear participants,

Those looking for supercomputing resources in your institution (High Performance Computing Cluster (HPC)), please reach out to their admin via call and email. As a registered student of the below listed institution, you can use the preinstalled Gaussian on their supercomputer at zero price.

S. No.	Institution	Weblink
1	IIT Kharagpur	➢ http://www.hpc.iitkgp.ac.in/
2	IIT Bombay	➢ https://www.cc.iitb.ac.in/page/services-software
3	IIT Madras	➢ https://hpce.iitm.ac.in/
4	IIT Kanpur	➢ https://www.iitk.ac.in/cc/softwares
5	IIT Delhi	➢ https://supercomputing.iitd.ac.in/?soft
6	IIT Guwahati	➢ https://www.iitg.ac.in/tamalb/karp/namd/out.html ➢ https://www.iitg.ac.in/tamalb/karp/namd/param.html
7	IIT Roorkee	➢ https://iitr.ac.in/Centres/Institute%20Computer%20Centre/Software.html ➢ https://hpc.iitr.ac.in/
8	IIT Ropar	➢ https://www.iitrpr.ac.in/it/assets/files/HPC_user_manual%20.pdf
9	IIT Bhubaneswar	➢ ----------
10	IIT Gandhinagar	➢ https://istf.iitgn.ac.in/hpc/paramananta.php
11	IIT Hyderabad	➢ ----------
12	IIT Jodhpur	➢ https://cc.iitj.ac.in/hpc/
13	IIT Patna	➢ ----------
14	IIT Indore	➢ http://iac.iiti.ac.in/assets/files/facilities/F35_CH_High_Performance_Computing_Facility.pdf
15	IIT Mandi	➢ https://research.iitmandi.ac.in/hpc/
16	IIT Varanasi	➢ https://www.iitbhu.ac.in/cf/scc
17	IIT Palakkad	➢ https://www.iitpkd.ac.in/hpc
18	IIT Tirupati	➢ ----------
19	IIT Dhanbad	➢ https://people.iitism.ac.in/~research/files/HPC_Brochure.pdf
20	IIT Bhilai	➢ ----------
21	IIT Dharwad	➢ https://www.iitdh.ac.in/high-performance-computing#:~:text=The%20HPC%20(AnantGanak)%20consists%20of,with%20the%20following%20basic%20info.
22	IIT Jammu	➢ https://dc.iitjammu.ac.in/
23	IIT Goa	➢ https://hpc.iitgoa.ac.in/