1ST ONLINE HANDS-ON-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@trainingcacrdelhi.com

Date: 8th April – 14th April 2025

Timing: Morning Batch: 11:00 AM – 12:00 PM IST Or Evening Batch: 7:00 PM – 8:00 PM IST

[Online Live Sessions along with Complete Recordings]

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

***IIT and Central Universities Students 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 Hands-on 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

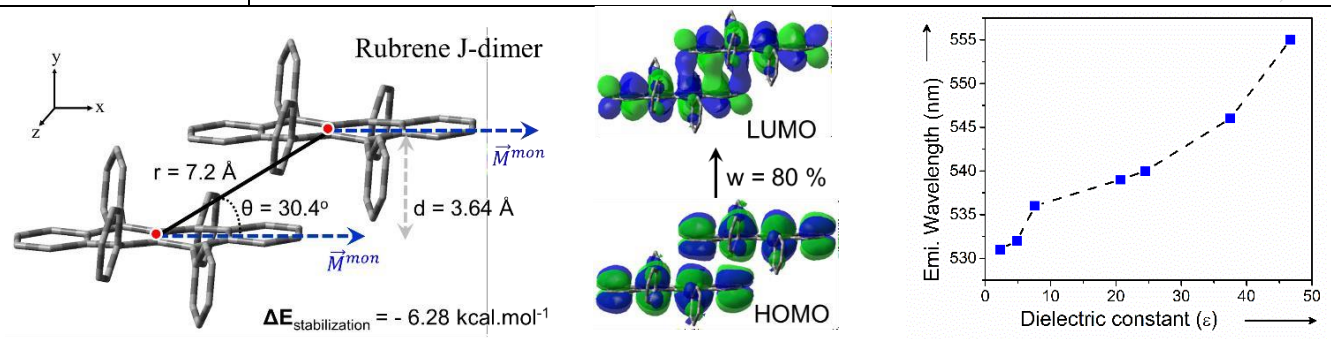
https://www.cacrdelhi.com/event-details/7-days-online-hands-on-trainng-on-dft-modelling-at-molecular-level-using-gaussian-dft-g-2

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

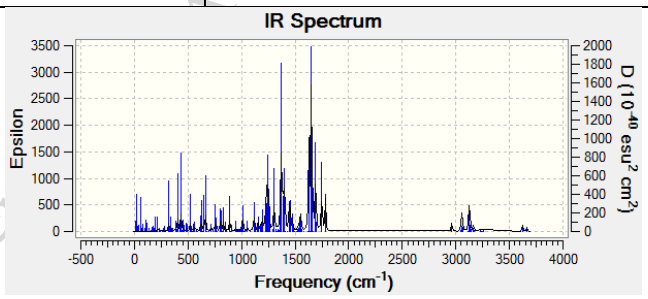
Join our WhatsApp Group

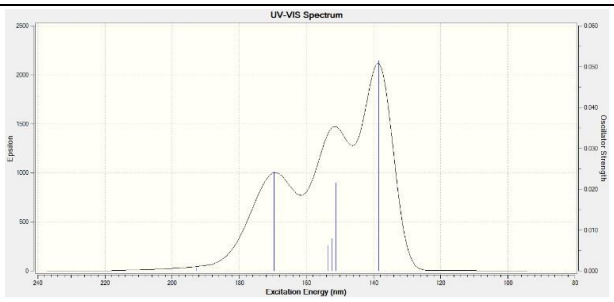
3. Detailed Day wise Schedule

8th April 2025 **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
9th April 2025 **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



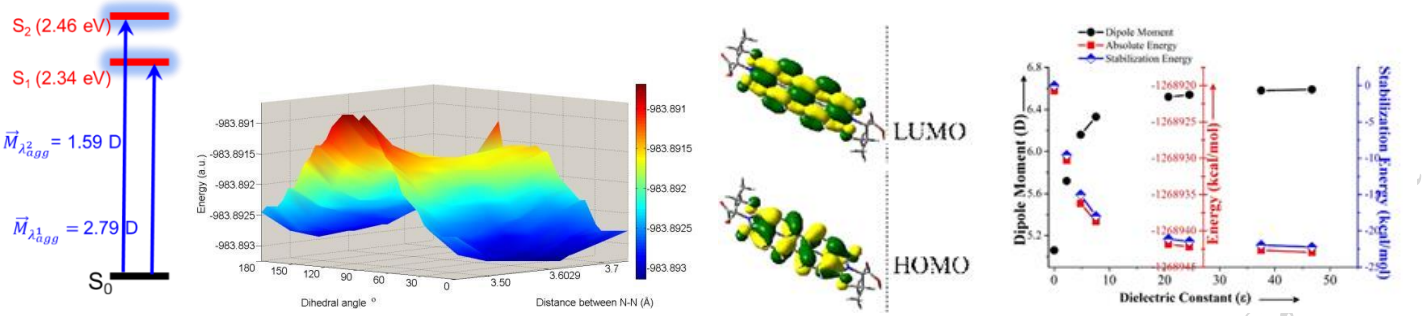
10th April 2025 **Day 3**	**Session 3: Frequency (Infrared Spectrum Computation)** Predict Stability, Dipole Moment Vector, Solubility, Vibrational frequencies (IR Spectrum), Visualization of Vibrational Modes:Stretching vs. Bending, Asymmetric vs. Symmetric Stretching, Negative Frequencies Frequency Shift on: Intermolecular interaction, Adsorption of molecule on surface, Metal Complexation
11th April 2025 **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



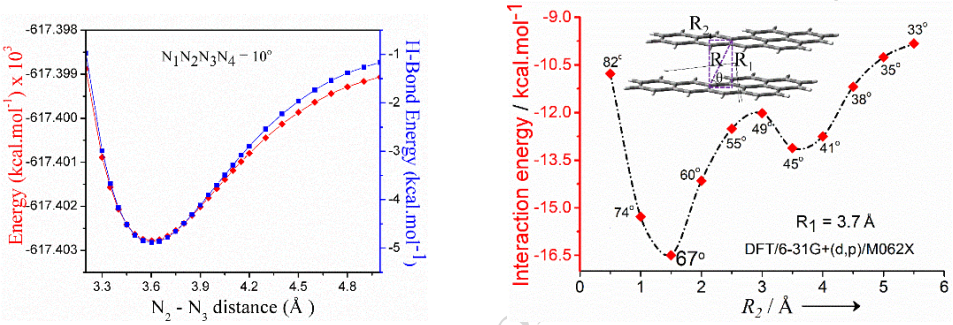


12th April 2025 **Day 5**	**Session 5: NMR Spectrum Computation** Hardness, Softness, Chemical Potential, Electronegativity and Electron Affinity, NMR Spectrum Calculation (C^{13}, H^1), Chemical Shift.

13th April 2025 **Day 6**	**Session 6: Adsorption (Intermolecular Interactions)** Adsorption: Intermolecular interactions between Adsorbate and Adsorbent, Single-Point Energy, Potential Energy Surface Diagrams, Optimized Binding Distances



14th April 2025 **Day 7**	**Session 7: Chemical Reaction** Reaction Mechanism, Enthalpy of reactions: Exothermic vs. Endothermic, Transition State Structures, Activation Energy, Intermediates



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	Rs. 2,500
Non-Indian Participants	Rs. 4100 or USD 48

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 600+ International and National participants of our previous workshops. The Centre previously had 5 invited lectures:

A. Dr. Snehasis Daschakraborty, Asst. Prof. (IIT Patna):[https://www.youtube.com/watch?v=CaZl0iFJU-I]

B. Prof. T. P. Radhakrishnan, Prof. (Hyderabad University):[https://www.youtube.com/watch?v=5IWNLsntgSU]

C. Dr. V. Ramanathan, Asst. Prof. (IIT BHU): [https://www.youtube.com/watch?v=erKb3y71VN8]

D. Prof. Kalidas Sen, Prof. (Emeritus) (Hyderabad University):[https://www.youtube.com/watch?v=jkz_Hb99vEg]

E. Dr. Ranganathan Subramanian, Associate Professor (IIT Patna)

Contact at

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

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/