Workshop Details

This workshop offers lectures and hands-on practice seasons on basic quantum mechanics and it's application to different chemical problems. Fundamentals of Python programming under HPC environment to predict molecular structures and properties using global optimization techniques. Application of Machine learning (ML) techniques in computational chemistry and use of 3D QSAR modelling in drug discovery.

Organizing Committee

Patron: Prof. Arvind Choubey
             Director, NIT Durgapur
Chairman: Prof. S C Moi, HoD
             Chemistry, NIT Durgapur
Convenors:
   Dr. S Ghosal, NIT Durgapur
   Prof. A Ayyappan, IIT Kharagpur
   Dr. D R Banerjee, NIT Durgapur

Contact

sghosal.ch@nitdgp.ac.in
9705726162 / 9641027482

Organized by
Department of Chemistry
NIT Durgapur

NIT Durgapur is an Institution of National Importance under the Ministry of Education, GoI. It offers undergraduate, postgraduate courses as well as doctoral programmes in Engineering, Basic Science, Social Science and Management Studies. The Department of Chemistry is one of the oldest departments of NIT Durgapur sponsored by DST-FIST and it offers 2-years M.Sc, 5-years Integrated M.Sc and PhD programme in Chemistry. The department has a rich heritage of inspiring teaching and cutting edge research in the frontier areas of chemistry.

Sponsored by
National Supercomputing Mission (NSM), DST, GoI

NSM has been set up to provide India with supercomputing infrastructure to meet the increasing computational demands of academia and industry steered jointly by Department of Science and Technology (DST) and Ministry of Electronics and IT (MeitY) and implemented by C-DAC, Pune and IISc, Bangalore.

NATIONAL INSTITUTE OF TECHNOLOGY DURGAPUR

presents

A Hands-on WORKSHOP on

"Molecular Structure Prediction Through Global Optimization and Machine Learning Techniques"

Program Schedule:
1st - 5th March, 2024

Mode: Physical & online

Members

Prof. Apruba Kumar Patra
Prof. Milan Maji
Prof. Dipankar Sukul
Prof. Rajnarayan Saha
Dr. Sujit Sankar Panja
Dr. Jitamunyu Chakrabarty
Dr. Utpal Adhikari
Dr. Tanmoy Kumar Saha
Dr. Krishnendu Pal
Dr. Sourav Laha
Dr. Paresh Nath Chatterjee

Registration Details

Last date for Registration: **22/02/2024**

Registration Fee	
Faculty	INR 3000
Ph.D. Scholar	INR 2000
PG/UG Student	INR 1000
Industry	INR 4000

Registration fee includes participation in all lecture and hands-on sessions, workshop materials and working lunch for all days.

Bank details for registration:

Bank Name: State Bank of India
Branch: R.E. College Durgapur
Beneficiary Name: CEP NIT DUGAPUR
A/C No: 37850318679
IFSC Code: SBIN0002108
MICR Code: 713002204

Registration Link :

https://forms.gle/m412xXVTv5gtWTHN8

Resource Persons:

Prof. Anoop Ayyappan, IIT Kharagpur
Prof. Biswarup Pathak, IIT Indore
Dr. Sandeep Kr. Reddy, IIT Kharagpur
Dr, Amit Kumar Paul, NIT Meghalaya
Dr. Subhas Ghosal, NIT Durgapur
Dr. Deb Ranjan Banerjee, NIT Durgapur

Program Schedule

Day 1 (1st March, 2024)

Lecture & Hands-on Season	
9.30 - 10.30 AM	Inauguration
10.30 - 11.00 AM	Tea-break
11.00 AM - 1.00 PM	Lecture
1.00 - 2.30 PM	Lunch & Discussion
2.30 - 4.00 PM	Hands-on practice
4.00 - 4.15 PM	Tea-break
4.15 - 5.30 PM	Hands-on practice

Day 2 (2nd March, 2024)

Lecture & Hands-on Season	
9.30 - 11.00 AM	Lecture
11.00 - 11.30 AM	Tea-break
11.30 AM - 1.00 PM	Lecture
1.00 - 2.30 PM	Lunch & Discussion
2.30 - 4.00 PM	Hands-on practice
4.00 - 4.15 PM	Tea-break
4.15 - 5.30PM	Hands-on practice

Day 3 (3rd March, 2024)

Lecture & Hands-on Season	
9.30 - 11.00 AM	Lecture
11.00 - 11.30 AM	Tea-break
11.30 AM - 1.00 PM	Lecture
1.00 - 2.30 PM	Lunch & Discussion
2.30 - 4.00 PM	Hands-on practice
4.00 - 4.15 PM	Tea-break
4.15 - 5.30 PM	Hands-on practice

Day 4 (4th March, 2024)

Lecture & Hands-on Season	
9.30 - 11.00 AM	Lecture
11.00 - 11.30 AM	Tea-break
11.15 AM - 12.45 PM	Lecture
12.45 - 2.30 PM	Lunch & Discussion
2.30 - 4.00 PM	Hands-on practice
4.00 - 4.15 PM	Tea-break
4.15 - 5.30 PM	Hands-on practice

Day 5 (5th March, 2024)

Lecture & Hands-on Season	
9.30 - 11.00 AM	Lecture
11.00 - 11.15 AM	Tea-break
11.15 AM - 12.30 PM	Hands-on
12.30 - 1.00 PM	Valedictory Season
1.00 PM -	Lunch