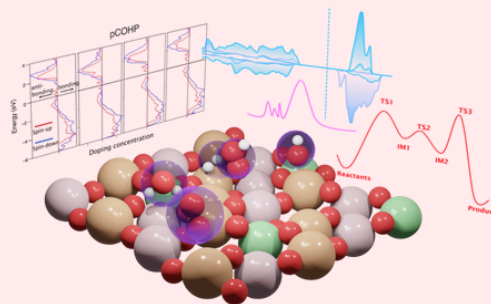


INDO-POLISH Workshop on Electronic Structure Calculations and Visualization with Molecular Nodes

Organizers



The Indian Institute of Petroleum and Energy, Visakhapatnam, AP, India, jointly with the Gdańsk University of Technology, Poland, is organizing a hybrid workshop on “Electronic Structure Calculations and Visualisation with Molecular Nodes” from 30th July to 3rd August 2024.

The workshop plans to cover ground-state electronic structure via advanced techniques such as Density Functional Theory (DFT). DFT has become an important tool in the area of materials research to understand the properties of materials, complement/understand experimental results, and design new materials.

Who can participate:

Motivated Postgraduate students, Research scholars, Postdoctoral fellows and Faculty of chemistry and allied areas who wish to pursue research in Electronic Structure Calculations.

Maximum number of Participants ~60

Registration Fee including GST:

Faculty: 5000 ₹	Faculty: 60 \$
Postdoc: 3000 ₹	Postdoc: 40 \$
PhD: 2200 ₹	PhD: 30 \$
M.Sc. Students: 1800 ₹	Students: 25 \$



Scan QR code or
use the link below
to register

<https://forms.gle/np6nbTuD5vEMLANCA>

Note:

- Payment link will be sent through an email to the selected candidates after successful registration.
- Accommodation will be provided based on availability at IPE Hostels (Rs 100/- per day on sharing basis for students)

30th to 3rd 2024
JULY AUGUST

Venue Address:
Indian Institute of Petroleum and Energy,
Visakhapatnam- 530003

Support emails: escvm_2024@iipe.ac.in,
chchgupta.chm@iipe.ac.in, subsappa@pg.edu.pl

The morning sessions of the workshop will consist of lectures on the basic principles and methodologies followed by research talks (covering experimental and theoretical aspects) showing their applications. The afternoon sessions will consist of hands-on tutorials where the participants will do simple calculations using the open source codes.

Further, we focus on scientific illustrations via Blender software with the recent concept of molecular nodes.

★ **Pre training for two days (Online)**
Training on LINUX OS, Plotting softwares, Script writing, Python language

Topics to be covered

Ground State Quantum Mechanics

Geometry optimisation

Potential energy surface

Intrinsic reaction coordinate

Molecular Orbitals and its visualisation

Excited State Quantum Mechanics

IR/Raman Spectra

TDDFT

Excited State Optimisation

Excited state PES

Quantum Dynamics

Potential energy surface

Reaction Mechanism

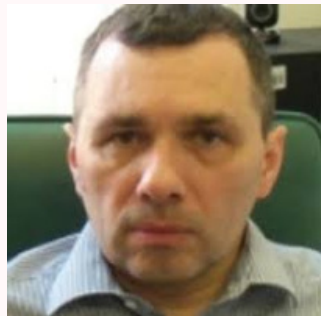
Visualisation

On Open Source Software's/Codes

Speakers



Prof. T. P. Radhakrishnan
University of Hyderabad
India



Prof. Maciej Bagiński
Gdańsk University
of Technology
Poland



Prof. Debashree Ghosh
IACS-Kolkata
India



Dr. Miłosz Wieczór
Gdańsk University
of Technology
Poland



Dr. Naveen Dandu
University of Illinois Chicago
USA



Dr. Subrahmanyam Sappati
Gdańsk University
of Technology
Poland



Dr. Tapta Kanchan Roy
Central University of Jammu
India



Dr. Tammineni Rajagopala Rao
IIT Patna
India



Dr. Rajagopala Reddy Seelam
Central University of Rajasthan
India



Dr. Nagaprasad Reddy Samala
Bar-Ilan University
Israel



Dr. Sridhar Palla
IIPE-Visakhapatnam
India



Dr. Ch Gupta Chandaluri
IIPE-Visakhapatnam
India



Mr. Rafeeqe Mavoore
SCIENTIFIC ILLUSTRATOR
SCIDART ACADEMY



Dr. Amit Sahu (TA)
Université de Bourgogne
France



Dr. Mateusz Kogut (TA)
Gdańsk University
of Technology
Poland

Organizing Committee

Chief Patron

Prof. Shalivahan, Director, Indian Institute of Petroleum and Energy (IIPE)

Patron

Prof. K. Vijaya Kumar, DoRD, IIPE

Patron from Gdańsk University of Technology, Poland

Prof. Maciej Bagiński, Department of Pharmaceutical Technology & Biochemistry

Convener

Dr. Ch Gupta Chandaluri, Assistant Professor, Chemistry, IIPE

Convener from Gdańsk University of Technology

Prof. Jacek Czub, Head of the Department of Physical Chemistry

Dr. Subrahmanyam Sappati, Assistant Professor (Tenure track), DPTB

Members

Dr. P. Aparoy, Associate Professor, IIPE

Dr. Sridhar Palla, Assistant Professor, IIPE