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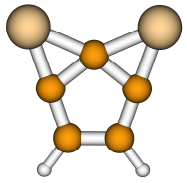
Organizers:

Mr. Debasish Bhattacharya

Scube Scientific, New Delhi.

Dr. S.K. Ashok Kumar and Dr. Thirumoorthy K
Department of Chemistry, SAS, VIT, Vellore



About VIT

VIT was established by Dr. G. Viswanathan, Chancellor in 1984 with the aim of providing quality higher education on par with international standards. VIT persistently seeks and adopts innovative methods to improve the quality of higher education on a consistent basis. The global standards set at VIT in the field of teaching and research spur us on in our relentless pursuit of excellence. Our Memoranda of Understanding with various international universities are our major strength. They provide for an exchange of students and faculty and encourage joint research projects for the mutual benefit. Many of our students, who pursue their research projects in foreign universities, bring high quality to their work and esteem to India and have done us proud. Recently VIT has been recognized as Institution of Eminence (IoE) by Government of India.

About SCUBE

It is a renowned distributor of leading-edge scientific software in the field of Computational Chemistry, Biology, Mathematical Modeling, Statistical Analysis, Data Mining and Market Research, collaborating with a wide range of companies across the globe such as Gaussian Inc, Wolfram Research Inc and PerkinElmer Informatics to name a few. Scube Scientific Software Solutions Pvt Ltd is proud to announce that it has been awarded the Quality in Business Certification from the International Trade Council.

VIT®
Vellore Institute of Technology
(Deemed to be University under section 3 of UGC Act, 1956)

SCUBE

Two days webinar on "**Gaussian, ChemDraw and Mnova Software**" in Collaboration with Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology and Scube Scientific

(21st and 22nd July 2020)

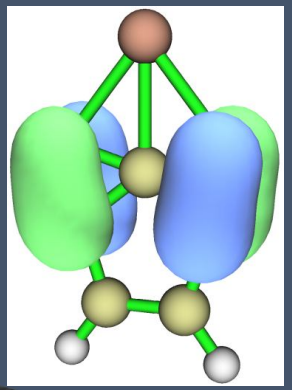
Resource Persons

Dr. Sourab Sinha received his PhD degree from Gauhati University, Assam. His study was based on QM/MM studies of Drug-DNA alkylation using computational methods. During his PhD, he was also selected for fellowship in The Petroleum Institute, Khalifa University, Abu Dhabi where he continued his research sponsored by ADNOC. Thereafter, he worked as a postdoctoral fellow at University of Szeged, Hungary.

Mr. Charitra Gour received his Master Degree in Pharmacy (Pharmaceutical Chemistry) from Amity University, Noida. He is currently working as a Technical Consultant for high-end scientific software like Gaussian, Ligandscout, Mnova, etc. at Scube Scientific Software Solutions, New Delhi

About Webinar

This webinar aims to help graduate students, and researchers to use computational chemistry tools in the most effective way. Computational chemistry is one of the fields of physical science which utilizes the modern computational techniques and hence this webinar is suitable for the new comers who have keen interest with quantum chemical calculations. Computational chemistry is rapidly expanding with the explosive growth of computational power. It is widely used in research and more interestingly in interdisciplinary research involving chemical and physical sciences, and biology.



Webinar Schedule – Day 1 (21st July 2020)

10:00 AM – 11:15 AM Gaussian

Introduction to Gaussian, Methodologies and Basis sets.

11:30 AM – 01:00 PM Gauss View

GaussView, Building Structures, Ground and Transition State Optimization, Frequency Calculations

02:30 PM – 04:00 PM

Intrinsic Reaction Coordinates, Redundant Coordinates, ONIOM, Solvation Models.

Webinar Schedule – Day 2 (22nd July 2020)

10:00 AM – 11:15 AM Chemdraw

Drawing Complex Diagram and Structures, Structure to Name, Name to Structure, Hot Keys, NMR Spectra Prediction, HELM and Biopolymer, Chemical Search with ChemACX, Chem 3D, Signals Notebook.

11:30 AM – 01:00 PM Mnova

Processing/Analysis and Reporting 1D and 2D NMR Spectra, Mass/TIC processing and analysis, Molecule Editor, Prediction of spectra of compound, Assignment, Structure elucidation from 1D and 2D data of the compound.

02:30 PM – 04:00 PM Gaussian

Scan Coordinates, UV calculations, Nuclear Magnetic Resonance, Stability.

Please click on the link below for:

Registration Deadline: 11:00 AM, 20th July, 2020

Feedback 05:00 PM, 22nd July to 02.00 PM, 23rd July, 2020

Participants will receive their e-Certificates by 25th July, 2020.