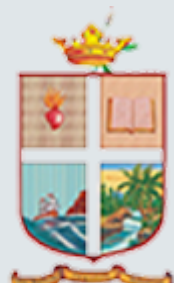




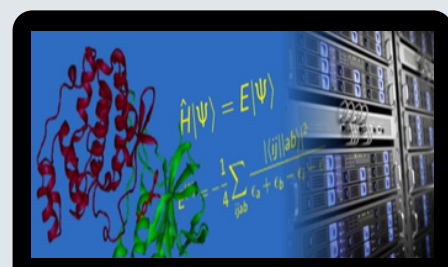
SACRED
HEART
COLLEGE
Autonomous



Department of Chemistry

Organizes

22nd PROF. K.V. THOMAS ENDOWMENT FACULTY TRAINING WORKSHOP



in

Computational Quantum Chemistry for Post Graduate Chemistry Courses in Indian Universities



13th and 14th October 2023



9.30 AM - 4.30 PM



Chavara IT Centre, Sacred Heart College Thevara,
Kochi

Key Features of the workshop

- *Exclusive Hands on Training using Free Softwares with Graphical User Interface and PC's/Laptops.*
- *Teachers, Research Scholars and Students from any chemistry background can attend.*
- *Essential Theory Coverage using simple approaches.*
- *The admission to the workshop is limited to 50 no's and will be on the basis of "first come, first serve"*



Rev. Dr. Jose John CMI
Principal

Dr. Franklin J
Head Of the Department

Dr. Abi T G
Convenor

Workshop Details

Modules Covered & Schedule	
Day1 : 13th October 2023 9.30 AM – Inauguration FN- Theory Sessions :10. AM – 1 PM 1.Introduction to Computational Quantum Chemistry 2. Hartree Fock Theory & Basis Sets in Computational Calculations 3. Introduction to Density Functional Theory AN-Practical Sessions: 2 to 4.30 PM 1. Chemical Structure Coordinates-Z Matrix 2. Quantum Chemistry Calculations using GAMESS-Firefly	Day2 : 14th October 2023 FN- Practical Sessions :9.30. AM – 1 PM 1. Calculations of fundamental constants in Organic Chemistry 2. Molecular Orbital Calculations AN-Practical Sessions: 2 to 4.30 PM 1. Thermodynamic Calculations 2. Reaction Mechanism Studies

Relevance of the Workshop

Computational chemistry course is implemented to the MSc Chemistry syllabus as a credit course of major universities in India especially in Kerala for the last 15 years. Though computational chemistry is accessible to higher level researchers, the essential theory and the practical skills in the area are not properly conveyed to post graduate students and college teachers of chemistry in India. Since this is not a traditional course like other core courses in physical chemistry, it is necessary to provide adequate training for the teachers and the students who have interest in computational techniques. To address the issue we organizes a two-day Hands on Faculty Training Workshop for selected and restricted number of participants on the topic "Computational Quantum Chemistry"

Resource Persons



Dr. Jayasree E G,
Professor,
Dept. of Applied Chemistry,
Cochin University of Science
And Technology

Dr. Jayasree E. G. did her Ph.D. in computational chemistry from Central University of Hyderabad. She did her post doctoral research in University of California, Berkeley and worked in National Science Foundation (NSF) funded project. She also worked in Trinity University, San Antonio, Texas and was involved in Welch funded research project. She was a faculty in University of Kerala during 2012-2022.



Dr. Abi T G
Assistant Professor
Dept. of Chemistry
Sacred Heart College, Thevara

Dr. Abi T G. did his Ph.D. in computational chemistry from IIT Kharagpur. He conducted several training workshops in Computational Chemistry including Science Academics Lecture Workshop in Computational Quantum Chemistry organized by Indian Academy of Sciences in 2017 at SH College Thevara. He is also the coordinator of UGC approved certificate course in computer aided drug design.

Registration Details :

Pay the fee & Register Using the link given below

<https://forms.gle/Mcfn1tPrpvqjA8287>

The registration fee Rs 1000 should be remitted to

***The Principal, Sacred Heart College.
Bank Account No: 17530100001012,
IFSC code: FDRL0001753,
Bank Name and Branch: Federal Bank, Thevara Branch***

Organizing Committee

***Prof. K V Thomas (Former HOD Chemistry & Union Minister)
Fr. Dr. Varghese Kachappilly CMI, Manager
Fr. Dr. Jose John CMI, Principal
Fr. Dr Joseph Varghese CMI, Vice Principal
Dr. Franklin John (Head of the Department)
Dr. Jinu George
Dr. Grace Thomas
Dr. Ignatious Abraham
Dr. Midhun Dominic C D***

***Mr. Senju Devassykutty
Dr. June Cyriac
Dr. Ramakrishnan S
Dr. Abi T G (Convenor)
Dr. Ammu Rosin Jose
Dr. Deepak D Prabhu
Dr. Jaison M J
Dr. Thomasukutty Jose
Dr. Shalumon K T***

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