

Registration Form

Name (Prof./Dr./Ms./Ms) _____

Designation _____

Organization _____

Address _____

Phone _____

E-mail _____

Date _____

Accommodation required _____

Note:
There is no registration fee for participation. Since the total no. of participants are limited to 100, those who wish to participate should register their names at the earliest. College Teachers and Research Scholars will get the preference for participation. Kindly send the filled-in registration forms by e-mail (scanned form) or in person on or before 31-12-2016 to the coordinator. Lunch and refreshments will be provided. Participants are requested to bring their laptop if possible. Those participants who need accommodation should inform the coordinator.

Organizers
General Convener : Prof. E. D. Jemmis (Dept of Inorganic and Physical Chemistry IISc Bangalore)
Coordinator : Dr. Abi T G (Sacred Heart College Thevara)
Dr. Joseph John (H&D Chemistry, Sacred Heart College Thevara)

All correspondence shall be addressed to
Dr. Abi T G
Coordinator, Science Academics Lecture Workshop,
Department of Chemistry, Sacred Heart College (Autonomous), Thevara - 682 013
Tel: 0464-2063190; Mobile: 9446055463; Email: abigt@shcollege.ac.in

Indian Academy of Sciences



In Association With
Post Graduate & Research Department Of Chemistry,
Sacred Heart College (Autonomous) Thevara



Organize
**Science Academics Lecture Workshop on
"Computational Quantum Chemistry"**

5th-7th January 2017

Venue : Fr. Melesius Hall & Computer Science Laboratory,
Sacred Heart College Thevara

INDIAN ACADEMY OF SCIENCES

The Indian Academy of Sciences (IAS), Bangalore founded in 1943 by Sir C. V. Raman, aims at promoting the progress and upholding the cause of science in pure and applied branches. The Academy's activities include publication of scientific journals and special volumes, recognition of scientific talent and improvement of science education. As part of the science education programmes the Indian Academy of Sciences, Bangalore in association with Indian National Science Academy (INSA), New Delhi and The National Academy of Sciences, India, Allahabad organizes programmes for the improvement of science education in Universities and colleges throughout the country.

SACRED HEART COLLEGE (AUTONOMOUS) THEVARA

Sacred Heart College, Thevara is an autonomous college in Kerala affiliated to M.G.J. University, Kottayam. The college was established in the year 1944 by the Carmelites of Mary Immaculate (CMI). It was originally affiliated to University of Madras. The college is ideally situated, on a peninsula strip known as Thevara, in the city of Kochi. The Vembanad Lake adds to the beautiful ambience of the campus. In the year 2000, the college was accredited by the National Accreditation and Assessment Council (NAAC) at the Five Star level, and in 2013 it was re-accredited at the A level. As a growing glory for its history of academic and non-academic achievements, the institution obtained Autonomous status in June 2014.

Post Graduate & Research Department of Chemistry.

The Department of Chemistry was established in 1944. This year Department is celebrating its Platinum Jubilee. It offers one undergraduate programme and two post graduate programmes (Chemistry & Pharmaceutical Chemistry). The Department is a recognized research center under Mahatma Gandhi University and it is now supported by DST under FIST programme.

About the Lecture Workshop

Computational chemistry is implemented as an inevitable topic for MSc Chemistry courses of different Universities of Kerala for the last few years. However the essential theory and the practical skills in computational chemistry are not properly conveyed to teaching-learning community. And since this is not a traditional course like other core courses in physical chemistry, it is necessary to provide adequate training for the faculty members, research scholars and students who have interest in computational chemistry. The three day lecture workshop is intended to arrange as a training program in the area of computational quantum chemistry for college teachers and research scholars. The workshop is a combination of lecture and practical sessions. On behalf of the Indian Academy of Sciences and Dept of Chemistry we cordially invite you to this workshop.

Programme Schedule

| 05-01-2017 (Thursday) | |
|---|--|
| 08.30 - 09.00 am | Registration |
| 09.00 - 09.30 am | Registration |
| 09.30 - 11.30 pm | Key Note Address |
| Topic | Introduction to Computational Quantum Chemistry Prof. E. D. Jemmis (IISc Bangalore) |
| 11.30 am | Tea Break |
| Lecture I & II (11.45 am - 02.50 pm) | |
| Topic | Hartree Fock Theory and SCF Procedure Dr. R. S. Swathi (IISER Trivandrum) |
| 01.00 pm | Lunch Break |
| Lecture III - Practical Section (02.30 pm - 04.30 pm) | |
| Topic | Computational Chemistry Practicals using a Personal Computer and Free Software. Dr. Abi T. G. (Sacred Heart College Thevara) |
| 06-01-2017 (Friday) | |
| Lecture IV & V (09.30 am - 12.00 pm) | |
| Topic | Basis Sets used in Computational Chemistry Calculations Dr. Parameswaran Panjath (NIT Calicut) |
| 10.45 am | Tea Break |
| Lecture VI & VII (12.00 pm - 02.30 pm) | |
| Topic | Introduction to Ab initio and Semi Empirical Methods in Computational Chemistry. Dr. G.N Sastri (ICT Hyderabad) |
| 01.00 pm | Lunch Break |
| Lecture VIII - Practical Session (02.30 pm - 3.30 pm) | |
| Topic | Computational Chemistry using Gaussian and Gauss View Programs Dr. M George (Sacred Heart College Thevara) |
| 07-01-2017 (Saturday) | |
| Lecture IX & X (09.30 am - 12.00 pm) | |
| Topic | Introduction to Density Functional Theory Prof. M.S Gopinathan (IISER Trivandrum) |
| 10.45 am | Tea Break |
| Lecture XI - Practical Session (12.00 pm - 01.00 pm) | |
| Topic | Computational Chemistry - Procedures and Practices Dr. M George (SH College Thevara) |
| 01.00 pm | Lunch Break |
| Lecture XII - Practical Session (01.30 pm - 03.30 pm) | |
| Topic | Introduction to Molecular Modeling Dr. Abi T. G. (SH College Thevara) |

**DEPARTMENT OF CHEMISTRY
SACRED HEART COLLEGE, THEVARA**

**REPORT
Of
Science Academics Lecture Workshop on
Computational Quantum Chemistry**

Date: 05-07 January 2017

Post Graduate and Research Department of Chemistry Sacred Heart College Thevara and Indian Academy of Sciences jointly organized Science Academics Lecture Workshop on “Computational Quantum Chemistry held at Computer Science Laboratory of the College on 05 to 07 January 2017.

The Program was a Three Day Hands on Training Lecture Workshop in Computational Chemistry for College Teachers. 100 Participants from various parts of the nation attended the workshop. Classes led by Fellows of Indian Academy of Sciences and experts in computational chemistry.

Prof ED Jemmis (Professor IISC Bangalore) was the convenor and Dr Abi T G (Assistant Professor, Sacred Heart College) was the coordinator.

PHOTO



Inauguration of Computational Quantum Chemistry Workshop by Rev. Dr. Jose Kuriedathu CMI on 05 January 2017

DEPARTMENT OF CHEMISTRY

SACRED HEART COLLEGE (AUTONOMOUS), THEVARA

FACULTY DEVELOPMENT PROGRAMME ON COMPUTATIONAL QUANTUM CHEMISTRY

05-07 February 2017

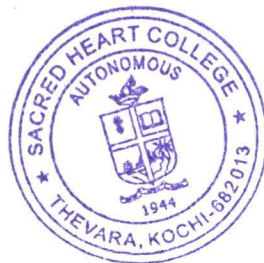
LIST OF PARTICIPANTS

| Sl. No. | Name | Institution |
|---------|---------------------|------------------------------------|
| 1. | A. Gopalakrishnan | DGV College, Chennai |
| 2. | Padmakumar K | Govt. College, Palakkadu |
| 3. | Tony Francis | St. Marys College, Manarcadu |
| 4. | Tijo Antony | Pavanathma College, Murickassery |
| 5. | Sarish S | NSS College, Pandalam |
| 6. | Monu Joy | MG University Kottayam |
| 7. | Paulcy Rani P R | Govt. College, Trivandrum |
| 8. | Suji C S | Govt. College, Trivandrum |
| 9. | Sujatha C V | Govt. College, Trivandrum |
| 10. | Deepa K | KAHM Unity College, Manjery |
| 11. | Shilpa Joy | KE College Mannanam |
| 12. | Sr. Gijimol | Alphonsa College, Pala |
| 13. | Elsy Shereena | MCC Calicut |
| 14. | Prajila M | University of Calicut |
| 15. | Rugmini Ammal | University of Calicut |
| 16. | Thomas V Mathew | St. Thomas College Pala |
| 17. | Jude Martin Mendes | St. Alberts College, Ernakulam |
| 18. | Savitha K U | NSS College, Chenganacherry |
| 19. | Roji J Kunnathu | Govt. College, Manimalakkunnu |
| 20. | Mathews K Manayani | Nirmala College Muvattupuzha |
| 21. | Remalekshmi Poduval | DB College Thalayolapparambu |
| 22. | Jalaja J Malayan | Baselius College, Kottayam |
| 23. | Suma Bino Thomas | Baselius College, Kottayam |
| 24. | Anjana V N | SSV College Valayanchirangara |
| 25. | Navya K N | SSV College Valayanchirangara |
| 26. | Anju Paul | SSV College Valayanchirangara |
| 27. | Ajmala Shireen P | Al Ameen College Aluva |
| 28. | Derry Holaday M G | St. Teresas College, Ernakulam |
| 29. | Anju Linda Varghese | Catholicate College Pathanamthitta |
| 30. | Zeena P Hamza | Maharajas College Ernakulam |
| 31. | Sudheesh N | NSS College Pandalam |



Jr. Johnson X Palackappan
Principal
Sacred Heart College (Autonomous)
Thevara, Kochi-682 013

| Sl. No. | Name | Institution |
|---------|------------------------|----------------------------------|
| 32. | Divya K M | NSS College Pandalam |
| 33. | Jolly V Antony | Maharajas College Ernakulam |
| 34. | Bindu Sharmila | Maharajas College Ernakulam |
| 35. | Fameeta Mary A G | Morning Star College Angamaly |
| 36. | Soumini C | CUSAT |
| 37. | Manu Kumar M N | Trivandrum |
| 38. | Anoop M R | St. Stephens College Pathnapuram |
| 39. | Priya Varma | Mercy College Palakkadu |
| 40. | Jibin K Varghese | DHSE Malappuram |
| 41. | Deepa K | KAHM Unity College, Manjery |
| 42. | Jenish Paul | UC College Aluva |
| 43. | Joseph George | SH College Thevara |
| 44. | Roy K B | SNGS College Pattamby |
| 45. | Dr. Joseph John | SH College Thevara |
| 46. | Dr. Jose K.B | SH College Thevara |
| 47. | Dr. Joseph T Moolayil | SH College Thevara |
| 48. | Dr. Thommachen Xavier | SH College Thevara |
| 49. | Dr. Sebastian V.S | SH College Thevara |
| 50. | Dr. George M | SH College Thevara |
| 51. | Dr. Jorphin Joseph | SH College Thevara |
| 52. | Dr. Franklin J | SH College Thevara |
| 53. | Dr. Jinu George | SH College Thevara |
| 54. | Dr. Grace Thomas | SH College Thevara |
| 55. | Dr. Ignatious Abraham | SH College Thevara |
| 56. | Mr. Midhun Dominic C D | SH College Thevara |
| 57. | Mr. Senju Devassykutty | SH College Thevara |
| 58. | Dr. June Cyriac | SH College Thevara |
| 59. | Dr. Ramakrishnan S | SH College Thevara |
| 60. | Dr. Abi T G | SH College Thevara |



Dr. Johnson X Palackappillil
Principal
Sacred Heart College (Autonomous)
Thevara, Kochi-682 013