



**SEMINAR**  
ON



**SPECTROSCOPY  
AND  
DENSITY FUNCTIONAL THEORY**



*Jointly Organised by*

**Chemistry Department  
Union Christian College ,Aluva  
and**

**Indian Society of Analytical Scientists  
(ISAS) Kerala Chapter**

**21 SEPTEMBER 2023**

**THURSDAY**

**TIME : 9:30 AM**

**VENUE: T.B . NINAN HALL, UNION CHRISTIAN COLLEGE , ALUVA**

# ISAS Kerala Chapter

The Indian Society of Analytical Scientists (ISAS) was established in 1983 at Bhabha Atomic Research Centre, Mumbai with the aim of dissemination of scientific information in the field of Analytical Sciences. This professional body of Analytical Scientists in India is engaged in assessing and analysing the impact of measurement sciences in industry, academy, R & D and community. Over the years ISAS has organized more than 35 national and international conferences on various topics of interest to the scientific community, which were well attended by leading professionals, researchers, teachers and students in India as well as abroad. ISAS is committed to raise the level of knowledge and expertise of entire community of analytical scientists in our country. ISAS has more than 4000 life members and 10 chapters spread all over India. ISAS Kerala chapter is one of the most active and vibrant chapters of ISAS. In conformity with its mission to strengthen analytical science through integrated strategic agenda of research and development, human capital and infrastructure, ISAS Kerala chapter has been organising conferences/ workshop / seminars, etc. and promoting analytical science education in Kerala.

## Department of Chemistry, UC College, Aluva

The Department of Chemistry in the prestigious Union Christian (UC) College was initiated in 1926 from the very inception of the Science stream of the Intermediate Course in the College. Prof. T. R. Anantharaman was the founder Professor and Head of the Department. The B.Sc. course in Chemistry was started in 1953, the department moved to the present building in 1969 under the able leadership of Dr. A. M. Chacko and the PG course was started in 1982, Owing to the untiring efforts of the eminent faculty, the research activities gradually increased, and the department attained formidable reputation in the national scene as one of the finest schools of chemistry for graduation. The Department currently has well equipped laboratories with a large number of analytical equipments for academic and research activities. Consequently, the Mahatma Gandhi University recognized the department of chemistry as a Post Graduate Research Centre for Study of Chemistry in 1984. The department has distinguished itself as a centre for innovative and pioneering research in a wide range of areas in chemistry and chemistry interfacing with physical and biological sciences. It has attained the status of a DST-FIST Sponsored department by DST in 2010. Now the department is marching forward in newer areas of research and teaching with young and energetic faculty members who has industrial and academic exposure from premier institutes of India and abroad. Chemistry division offers research opportunities in a wide range of interest from traditional organic, bio-inorganic chemistry to new frontiers of material research, medicinal chemistry and nano science.

## Scope

Over the past few years, the educational seminars and workshops conducted by ISAS have become very popular and were well attended and appreciated. The success of these seminars encouraged ISAS to work with interested colleges and Universities in Kerala to replicate these courses in their premises. It is realized that there is a tremendous need for the education of theories of various analytical techniques, particularly advanced instrumental methods among the graduate and post graduate students. As a part of its commitment and constant endeavor to promote education in analytical science and technology, ISAS has now decided to organize an one day seminar on " Spectroscopy and Density Functional Theory" at Union Christian College, Aluva on 21st September 2023, which is also the formation day of ISAS Kerala Chapter.. This seminar will focus on the basics, technology and applications of Raman Spectroscopy and NMR spectroscopy. The seminar covers a lecture of Density Functional Theory, a most popular and versatile computational method used in physics, Chemistry and materials science to investigate the electronic structure.

## Registration

Those who are interested to participate in the seminar are requested to register. Registration is *free* for students, research scholars and teachers. Spot registration can also be made at conference venue on the seminar day.

## Organising Committee

Dr. M.I. Punnose, Principal, Union Christian College, Aluva - Patron  
Dr. Ragaw Saran, National President, ISAS – Patron  
Dr. Rajeev R., Chairman, ISAS Kerala Chapter- Patron  
Dr. V.R. Nair, Ex. Chief General Manager, Indian Rare Earth Ltd., Kollam  
Dr. N.K. Pillai, CEO, Kerala Enviroinfrastructure Ltd, Ambalamugal, Kochi  
Dr. K.K. Mohammad Yusuff, Vice President, ISAS  
Dr. S. Sugunan, Retired Professor, CUSAT, Kochi  
Dr. K.K.A. Rashid, Consultant, Active Charr Product, Kochi  
Dr. P.V. Joseph, Joint Treasurer, ISAS  
Ms. Smitha Roy, Department of Chemistry, Union Christian College, Aluva  
Dr. Simi Pushpan K., Department of Chemistry, Union Christian College, Aluva  
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Dr. Divya Susan Philips, Department of Chemistry, Union Christian College, Aluva  
Dr. A.C. Sunil Shekhar, Department of Chemistry, Union Christian College, Aluva

### Chairman

**Dr. P. Unnikrishnan**

Vice Chairman, ISAS-K  
Union Christian College, Aluva

### Co-Chairman

**Ms. Minu Joys**

Head, Department of Chemistry,

### Convener

**Dr. Jenish Paul**

Union Christian College

Contact: +919496462165

Email: [jemishpaul@uccollege.edu.in](mailto:jemishpaul@uccollege.edu.in)



# Programme Schedule

Inaugural Session 9:30 am to 10:00 am

## Technical session 1

10:00 am to 11:00 am

### Dr. Yoosaf Karuvath

Professor, Department of Applied Chemistry, CUSAT

**Topic: Raman Spectroscopy for Sensing and Diagnostics**

## Technical session 2

11:30 am to 12:30 pm

### Dr. Sindhu Mathai

Assistant Professor, Department of Applied Chemistry, CUSAT

**Topic: NMR Spectroscopy: Principles and Applications**

**Lunch Break** 12:30pm–1:30 pm

## Technical session 3

1:30 pm to 2:30 pm

### Dr. Jayasree Elambalassery

Professor, Department of Applied Chemistry, CUSAT

**Topic: Density Functional Theory – an efficient predictive tool for realistic systems calculations**

Valedictory function and Certificate distribution  
2:30 pm to 3:00 pm