

# SCIENCE ACADEMIES' EDUCATION PROGRAMME

SEP/LW/January/2017

04 November 2016

## JOINT SCIENCE EDUCATION PANEL

### Indian Academy of Sciences

Sebastian, K. L.  
(Chairman)  
Arunan, E.  
Bachhawat, A. K.  
Balakrishnan, V.  
Chattopadhyay, Nitin  
Dhar, Deepak  
Mukunda, N.  
Murthy, M.R.N.  
Radhakrishnan, T. P.  
Rangarajan, Govindan  
Saidapur, S.K.  
Sankaran, P.  
Satheesh, S.K.  
Sengupta, Pulak  
Subramaniam,  
Annapurni

### Indian National Science Academy

Chattaraj, P. K.  
Chattoo, B.B.  
Chaudhuri, Probal  
Goswami, J.N.

### The National Academy of Sciences, India

Dimri, V.P.  
Khurana, Paramjit  
Misra, Gadadhar  
Mittal, J.P.

### Contact Address

Mahabaleswara, T.D.  
Coordinator  
Refresher Courses &  
Lecture Workshops  
Indian Academy of  
Sciences  
P.B. No. 8005  
C.V. Raman Avenue  
Sadashivanagar P.O.  
Bengaluru 560 080  
India

### Telephone:

91-80-2266 1210  
91-80-2266 1222  
Fax:  
91-80-2361 6094

### Email:

sep@ias.ernet.in

Dr Abi T.G.  
PG & Research Dept. of Chemistry  
Sacred Heart College  
Thevara  
Kochi 682 013

Sub: Lecture Workshop on "Computational quantum chemistry" at Sacred Heart College, Thevara during 05-07 January 2017.

Dear Dr Abi,

This has reference to the letter forwarding a proposal and/budget for organizing a three-day Lecture Workshop in your College. The Joint Science Education Panel of the three Academies will be happy to sponsor and support the Lecture Workshop. We note that Prof. E.D. Jemmis (IISc, Bangalore) will be the Workshop Convener and that you will be the Workshop Co-ordinator.

(a) Your budget of Rs. 1,56,500/- for 100 participants (inclusive of travel expenses for Resource Persons) has been approved by the Science Education Panel.

(b) Please note that only the names of Convener and Coordinator of the Workshop should be included in brochure/invitation etc. Names of members of the management, organizing committees, patrons etc should be strictly avoided.

(c) Please ensure that the expenditure on individual items does not exceed the sanctioned BUDGET HEAD. If the actual expenditure exceeds the sanctioned budget, THE HOST INSTITUTION SHOULD TAKE CARE OF THE DIFFERENCE.

(d) Lecture Workshops are sponsored and supported by the three National Science Academies – IASc, INSA and NASI. The names of INDIAN ACADEMY OF SCIENCES (BENGALURU), INDIAN NATIONAL SCIENCE ACADEMY (NEW DELHI) and THE NATIONAL ACADEMY OF SCIENCES, INDIA (ALLAHABAD) should therefore be mentioned in all publicity material such as programme sheet, invitation cards, etc.

(e) It may be noted that no formal certificates should be issued to participants. A letter of attendance signed by Coordinator may be issued to those who need it.

(f) The Workshop should be called Science Academies' Lecture Workshop on "Computational quantum chemistry".

(g) You should send us three copies of the printed programme cards once it is printed.

(h) We can advance money by electronic transfer on a specific request



Indian Academy  
of Sciences,  
Bangalore



Indian National  
Science Academy,  
New Delhi



The National Academy  
of Sciences, India  
Allahabad

from you. We will need the following bank details:

1. Account No;
2. Name of the Account Holder;
3. Name of the Bank;
4. Name of the Branch;
5. IFS code for non-SBI accounts.

(i) The audited expenditure statement/utilization certificate duly signed by competent authority (CA or Financial Controller) to be sent along with the report, once the Course is over. This is required for the audit compliance.

You can go ahead with organizing the Workshop in consultation with Prof. E.D. Jemmis and keep in touch with us about the progress.

With regards,

Yours sincerely,



T. D. Mahabaleswara  
4/11/16

Coordinator (Lecture Workshop/Refresher Course)  
Science Education Panel

Total Revenue Generated under the consultancy of Dr. Abi T G, Asst. Prof. Chemistry as a coordinator and resource person in 2017 = Rs 1,56500

Dept. of Chemistry Federal Bank Account Pass Book Pages

		PHOTO	DEPOSIT PRODUCTS	
			Yuvamitra	
		Fixed Deposits		
		Cash Certificates		
		Federal Savings Fund/Fedjeevan		
		Suraksha Deposit		
		Current Deposit Account		
		Privilege Current Account		
Account Type	: Savings Account			
Account Number	: 17530100007050			
Customer ID	: 25252868			
Name	: M/S S H COLLEGE DEPT OF CHEMISTRY 2.MR JOSEPH JOHN 3.DR FRANKLIN J			
Address	: DEPARTMENT OF CHEMISTRY SH COLLEGE THEVARA ERNAKULAM-682013.INDIA			
Operational Instruction	: JOINT			
Date of Opening	: 03-09-2013			
Account activation date	: (For Pre-opened kits)			
Authorised Signatory :		ADVANCE PRODUCTS		
		Personal Loans		
		Personal Car Loans		
		Housing Loans		
		Kissan Credit Cards		
		Vanijya Loan		
		Gold Loans and many more		
		For details, please contact any of our branches visit <a href="http://www.federalbank.co.in">www.federalbank.co.in</a>		

Date	Description	Account No	Debit	Credit	Balance	Cr
08-10-16	SUBIN JOSEPH SEBA	10022993	20.000.00		1.70.402.00	Cr
10-11-16	JOSEPH JOHN	10022995	8.500.00		1.61.902.00	Cr
10-11-16	CASH			8.500.00	1.70.402.00	Cr
12-11-16	KGA HOTELS AND RE	10022994	1.00.000.00		70.402.00	Cr
17-11-16	NFT/INDIAN /SBIN9			1.17.400.00	1.87.802.00	Cr
24-11-16	ABI TG	10022996	20.000.00		1.67.802.00	Cr
06-12-16	THE PRINCIPAL SAC			44.600.00	2.12.402.00	Cr
12-12-16	17530100007050:In			1.781.00	2.14.183.00	Cr
13-12-16	ABI TG	10022997	20.000.00		1.94.183.00	Cr
15-12-16	MIDHUN DOMINIC	10022998	7.000.00		1.87.183.00	Cr
29-12-16	REJI JOSEPH	10022999	8.000.00		1.79.183.00	Cr
04-01-17	JOSEPH JOHN	10023001	16.000.00		1.63.183.00	Cr
10-01-17	RAMAKRISHNAN	10023005	24.000.00		1.39.183.00	Cr
11-01-17	THE WYTE FORT	10023004	2.352.00		1.36.831.00	Cr

11-01-17	SAJU A J. (PSJ 012)	10023002	15,000.00		1,21,831.00	Cr
11-01-17	DIRECTOR RENEWAL	10023003	23,000.00		98,831.00	Cr
20-01-17	THE DIRECTOR RENE	10023006	20,000.00		78,831.00	Cr
03-02-17	NFT/SBT PER/SBTR7			10,000.00	88,831.00	Cr
04-02-17	JOSEPH JOHN	10023007	15,000.00		73,831.00	Cr
04-02-17	JOSEPH JOHN	10023008	9,000.00		64,831.00	Cr
06-02-17	NFT/COCHIN /SBTR7			42,349.00	1,07,180.00	Cr
07-02-17	JOJI JOSEPH	10023009	36,500.00		70,680.00	Cr
10-02-17	ABI TG	10023010	5,800.00		64,880.00	Cr
10-02-17	NFT/COCHIN /IBKL1			25,000.00	89,880.00	Cr
14-02-17	PARTHASARATHY HAN	10023011	61,000.00		28,880.00	Cr
23-02-17	JOSEPH JOHN	10023012	20,000.00		8,880.00	Cr
06-03-17	17530100007050:In			1,178.00	10,058.00	Cr
04-04-17	CASH			15,000.00	25,058.00	Cr
17-04-17	CLG/CHEMIND/24175			15,000.00	40,058.00	Cr
17-04-17	CLG//381810/SOUTH			10,000.00	50,058.00	Cr

**SACRED HEART COLLEGE, THEVARA, COCHIN - 682 013**  
**LECTURE WORKSHOP ON " COMPUTATIONAL QUANTUM CHEMISTRY "**  
**HELD ON 5<sup>TH</sup> TO 7<sup>TH</sup> JANUARY 2017**

**STATEMENTS OF ACCOUNTS FOR THE PERIOD FROM 17.11.2016 TO 07.01.2017**

RECEIPTS	₹	PAYMENTS	₹
To Opening Balance	Nil	By <u>Workshop Expenses:-</u>	
" Amount Received from Joint Science Education Panel	1,17,400.00	Publicity Expenses	6,600.00
" Advance from Management	51,201.00	Registration and Stationery	10,200.00
		Food Expenses	66,500.00
		Honorarium for	
		- Resource Persons	24,000.00
		- Convener/Co-ordinator	4,500.00
		- Supporting Staff	2,000.00
		Boarding and Lodging Expense	12,352.00
		Travel Expenses	32,249.00
		Miscellaneous Expenses	10,200.00
		Closing Balance	Nil
<b>Total</b>	<b>1,68,601.00</b>	<b>Total</b>	<b>1,68,601.00</b>

**AUDITORS' REPORT**

Verified with the books of accounts produced before us and found correct according to the explanations given to us

Ernakulam  
18.01.2017



**CHARTERED ACCOUNTANTS**

**C. J. ROMID F.C.A**  
**Membership No: 22498**  
**Partner**

## Registration Form

Name (Prof./Dr./ Ms./ Mr) \_\_\_\_\_  
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** (HoD 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: 0484 2663180; Mobile: 9446058463; Email: abtgc@shcollege.ac.in

## Indian Academy of Sciences



Indian Academy of Sciences



Indian National Science Academy



The National Academy of Sciences

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



Organizes,

## Science Academics Lecture Workshop on "Computational Quantum Chemistry"

5<sup>th</sup>-7<sup>th</sup> 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 Academies' 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 (NSA), 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 MGS 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 peninsular 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 crowning 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 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 : Inauguration  
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 – 2.30 PM)

Topic: **Hartree Fock Theory and SCF Procedure**  
Dr R S Swathi (IISER Trivandrum)

1.00 PM: Lunch Break

Lecture III – Practical Section (2.30 to 4.30 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 (9.30 – 12.00 pm)  
Topic: **Basic Sets used in Computational Chemistry Calculations**  
Dr. Parameswaran Pattiyil (NIT Calicut)

10.45 AM – Tea Break

Lecture VI & VII (12.00 pm – 2.30 pm)  
Topic: **Introduction to Ab Initio and Semi Empirical Methods in Computational Chemistry.**  
Dr. G N Sastri (IICT Hyderabad)

1:00 PM: Lunch Break

Lecture VIII – Practical Session (2.30 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 – 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 – 1.00 pm)  
Topic: **Computational Chemistry - Procedures and Practises**  
Dr. M George (SH College Thevara)

1.0 PM: Lunch Break

Lecture XII: Practical Section (1.30 – 3.30 pm)  
Topic: **Introduction to molecular Modeling**  
Dr. Abi T. G., SH College, Thevara