Report on

Science Academies Lecture-Workshop

on "Beyond the Boundaries of Chemistry"

October 29th – 31st 2018

Organized by

Department of Chemistry
Providence Women's College
Calicut, Kerala – 673009

Convener

Dr. Swapan K Pati, FASc, FNASc, FTWAS
Professor and Chairman
Theoretical Sciences Unit,
JNCASR, Bangalore

Coordinator

Dr. Deepthi Jose,
Assistant professor,
Dept. of Chemistry,
Providence Women's College
Calicut, Kerala - 673009

The three-day lecture workshop on "Beyond the Boundaries of Chemistry" was sponsored by the three science academies, the Indian Academy of Sciences, Bangalore, Indian National Science Academy, New Delhi and the National Academy of Sciences, India, Allahabad was successfully organized and conducted by the Department of Chemistry, Providence Women's college during October 29th – 31st 2018. The aim of this workshop was to introduce various interdisciplinary fields like nanoscience, computational science, photochemistry, green energy technologies, drug design etc.to students and the researchers. Prof. Swapan K Pati, Professor and Chairman, Theoretical Science Unit, JNCASR Bangalore was the convener of the workshop and Dr. Deepthi Jose, Assistant Professor, Department of Chemistry, Providence Women's College, Calicut was the coordinator.

We had eminent scientists from premier science institutions in India as our resource persons. Our resource persons include 1) Prof. S. Ramasesha, IISc Bangalore 2) Prof. Sheela K Ramasehsa, NIAS Bangalore 3) Prof. Uday Maitra, IISc Bangalore, 4) Prof. P. K. Das, IISc Bangalore and 5) Prof. Raghu C. NIT Calicut. A total of 12 lectures were given by resource persons. About 150 participants (faculty, PG students, research scholars) from various institutions participated in this three-day lecture workshop.

Day 1: 29/10/18 (Monday)

The workshop commenced on October 29th 2018, with an inaugural ceremony. Dr. Gigy Abraham, H.O.D., Department of Chemistry welcomed the gathering. Dr. Minoo Divakaran, IQAC Coordinator, Providence Women's college presided over the inaugural ceremony. Prof. Swapan K Pati, Professor and Chairman, Theoretical Science Unit, JNCASR Bangalore and the convener, inaugurated the workshop. In his inaugural address he mentioned about the importance of getting exposed to various interdisciplinary fields and asked the participants to make complete use of the eminent resource persons who came to handle different sessions. He also outlined the various activities of Science academies and the purpose of this workshop. Prof. S. Ramasesha, Solid state and Structural Chemistry Unit, Indian Institute of Science, Bangalore offered his felicitations. Prof. Ramasesha talked about the science supporting activities of the academies like summer research fellowships for students and teachers, lecture workshops of 2- or 3-days duration for students and teachers, publication of a monthly journal of science education – Resonance etc. to nurture science all over the country. Dr. Deepthi Jose, coordinator of the workshop purposed the vote of thanks.

Inaugural Function (From left to right): Prof. Swapan K Pati, JNCASR Bangalore (Workshop Convener); Prof. S. Ramasehsa, IISc Bangalore; Prof. Uday Maitra, IISc Bangalore; Dr. Minoo Divakaran, IQAC coordinator, Providence Women's College; Dr. Gigy Abraham, HOD, Department of Chemistry, Providence Women's College; Dr. Deepthi Jose (workshop coordinator)

Dr. Minoo Divakaran delivering the presidential address and Prof. Swapan K Pati inaugurating the three-day lecture workshop

Prof. S. Ramasesha briefing the various science supporting activities of Science Academies

The first session on day 1 was handled by Prof. Uday Maitra on the topic 'Molecules that defy rules'. The session dealt with molecules that doesn't obey the principles and rules which are applicable to the majority of molecules and reactions. The nonexistence of four planar carbon bonds, some interesting molecules were all part of the lecture. Prof emphasized on the International Year of Periodic table to be held in 2019.

Prof. S. Ramsesha lead the second session of day 1 on 'Probing energy levels in molecules and solids'. The fundamental theoretical aspects of various spectroscopic techniques were discussed. The lecture included Born-Oppenheimer approximation, Frank Codon principle etc. in detail.

The afternoon session was made interesting by Prof. Uday Maitra on the topic 'Drug design- Is it really that easy'. The drugs that have hit the sales to about one million, the enzymatic activity of the drug were the main topics covered. The methods by which drugs get easily assimilated in the body using the principles of enzymatic mechanism formed the central theme of the lecture.

The last session on day 1was made informative by Prof. P. K. Das on 'Molecular Electronics'. The advancement of technology in producing miniature size devices, the usage of molecules in rectification were highlighted in the talk. The need for transition from electronics to photonics was emphasized in the lecture.


Prof. Uday Maitra talking on Molecules which Defy Rules and Prof. P. K. Das delivering his talk on Nanoelectronics.

Day 2: 30/30/18 (Tuesday)

We started our session III with the talk of Prof.Sheela K Ramashesha, from NIAS Banglore, about the relevant topic ‘Issues of Clean Energy’. Prof. Sheela started with the factors which increase the temperature. She talked about Greenhouse effect, cited many examples on this dangerous situation. And also talked about the pollution caused by burning fossil fuels by using vehicles. She also explained the fundamentals of semiconductors and solar technology. Audience was included in the interactive session.

The next talk was by our Convenor Prof.Swapan K Pati, from JNCASR Banglore on ‘Chemical Bonding to artificial atoms from Classroom Quantum Theory’. He talked about the basics of Quantum Mechanics as well as its higher levels and applications. His talk also included Chemical Bonding, Hyper conjugation and quantum dots.


Prof. Sheela K Ramasesha delivering talk on Issues of Clean Energy and Prof. Swapan K Pati on Chemical Bonding to Artificial Atoms from Classroom Quantum Theory

After the lunch break, we began our IV session. The first talk was led by Prof. P. K. Das from IISc Banglore on ‘Photo dissociation Dynamics’. He explained the process of understanding the rate of bond breaking by shining light on it and the underlying mechanism. The photodissociation dynamics was explained in detail through the developments in methyl iodide dissociation using ultraviolet radiation.

And the last talk of the day was presented by Prof.Swapan K Pati on ‘Modeling I to V characteristics of molecular systems. He discussed the fundamentals of doing electronics with molecules, how resistivity, conductivity definition change when one deals with single electron tunneling current, how molecules act as tunneling carrier for electron, quantization of current and how to obtain I-V characteristics of a single level molecule to multi-level complex molecular systems etc. Though the topic was a bit advanced, Prof. Swapan managed to make it simple by giving us some examples and even made us to think about aspects of what he was saying.

Day 3: 31/10/18 (Wednesday)

The session V on day 3 started with talk by Prof. Ramasesha on Probing Energy Levels in Molecules and Solids II. After briefing about his talk on day 1, Prof. Ramasesha moved to vibrational spectroscopy, followed by N.M.R spectroscopy. He also discussed Mossbauer spectroscopy. The session also covered the various applications of spectroscopy.

The second talk was by Prof. Raghu C on Computational Methods. Starting from the fundamentals, he explained the theory of Density Functional Theory and its applications. Prof. Raghu also mentioned about choosing the right functional for our system of interest and the precautions we should take while doing and analyzing DFT calculations.

The afternoon session was initiated with talk by Prof. Sheela K Ramasesha on Green Energy Technologies. She explained the details of tapping energy from solar energy, tidal energy, wind energy, hydroelectric power etc. The advantages and limitations of each of these methods was discussed. She elaborated the use of solar energy for running trains, cars, for making parking places etc.

The last session was led by Prof. Swapan K Pati, Prof. S. Ramasesha and Prof. Raghu C. Prof. Ramasesha outlined about the need of approximations in calculations and size constrain in quantum calculations. Prof. Swapan explain in detailed various approximations starting from Hartree-Fock to Configuration Interaction calculations. Advantages of each type of calculations and the systems which can be studied using these calculations were discussed. The concept of basis set was also elaborated in detail.

Prof. S. Ramasesha delivering talk on Probing Energy Levels in Molecules and Solids II and Prof. Raghu C. on Computational Methods

Prof. Swapan K Pati on Challenges in Computational Chemistry

The three-day lecture workshop was concluded with a valedictory function. Prof.Swapan K Pati urged students to ask questions about what they see and what they observe during his concluding remarks. He also advised the students to make the best use of the opportunities available in the present days and appreciated the efforts of the organizers for the successful conduct of the workshop. Participants were asked to give their feedback. A few participants from different colleges spoke about various aspects of the workshop. They felt this workshop was well organized and kept the time as per the schedule. They commented that some of the topics were advanced for post graduate and under graduate students. But the workshop introduced many new fields to them and thanked the opportunity to interact with eminent scientists. They suggested that this kind of workshop should be continued more in the near future. The feedback was positive and the workshop ended by appreciating the financial support and encouragement of Science Academies and also thanked for support and contributions by all in one way or other by the coordinator, Dr. Deepthi Jose.

Convener of the Workshop Prof. Swapan K Pati giving his Concluding remarks


Feedback session by the students

List of students and faculty members participated from various colleges

SI.No	Name of the College	No. of students	No. of research scholars	No. of teachers	Total
1	Farook College, Calicut	11	1	2	14
2	NIT Calicut		8		8
3	MAMO College, Mukkam	12			12
4	Govt. Arts and Science College, Calicut	15			15
5	Govt. College, Chittoor			1	1
6	Govt. Engineering college, Calicut			1	1
7	Malabar Christian College, Calicut	11	1	3	15
8	Zamorin's Guruvayurappan College	13	2	4	19
9	Kannur University		1		1
10	SES College, Sreekandapuram, Kannur			1	1
11	University of Calicut		1		1
12	Markaz Arts and Science College			1	1
13	Roche Diagnostics India Pvt Ltd		1		1
14	St. Joseph's College, Devagiri	1		2	3
15	Providence Women's College, Calicut	57			57
	Total	120	15	15	150

Workshop Announcement Brochure

DAY 2, 30th October 2018 (Tuesday)

Session III

9.30-10.45 am — Issues of Clean Energy
Prof. Sheela K. Ramasesha
National Institute of Advanced Studies(NIAS), Bangalore
Discussion

10.55-11.15 am — Tea break

11.15-12.30 pm — Chemical Bonding to Artificial Atoms from Classroom Quantum Theory
Prof. Swapan K Pati
JNCASR Banglore
Discussion

12.40- 2.00 pm — Lunch break

Session IV

2:00 – 3:15 pm — Photodissociation Dynamics
Prof. P. K. Das
Indian Institute of Science, Bangalore
Discussion

3:25 -3: 35 — Tea break

3.35-4.50 pm — Modeling I-V Characteristics of Molecular Systems
Prof. Swapan K Pati
JNCASR Banglore
Discussion

DAY 3, 31st October 2018 (Wednesday)

Session V

9.30-10.45 am — Probing Energy Levels in Molecules and Solids II
Prof. S. Ramasesha
Indian Institute of Science, Bangalore
Discussion

10.55-11.15 am — Tea break

11.15-12.30 pm — Computational Methods
Prof. Raghu C., NIT Calicut
Prof. Swapan K Pati, JNCASR Banglore
Discussion

12.40 – 2:00 pm — Lunch break

Session VI

2.00- 3:15 pm — Green Energy Technologies
Prof. Sheela K. Ramasesha
National Institute of Advanced Studies(NIAS), Bangalore
Discussion

3.25-3.35 — Tea break

3.35-4.50 pm — Challenges in Computational Chemistry
Prof. Raghu C., NIT Calicut
Swapan K Pati, JNCASR Bangalore

5.00 – 5.15 pm — Valedictory Session

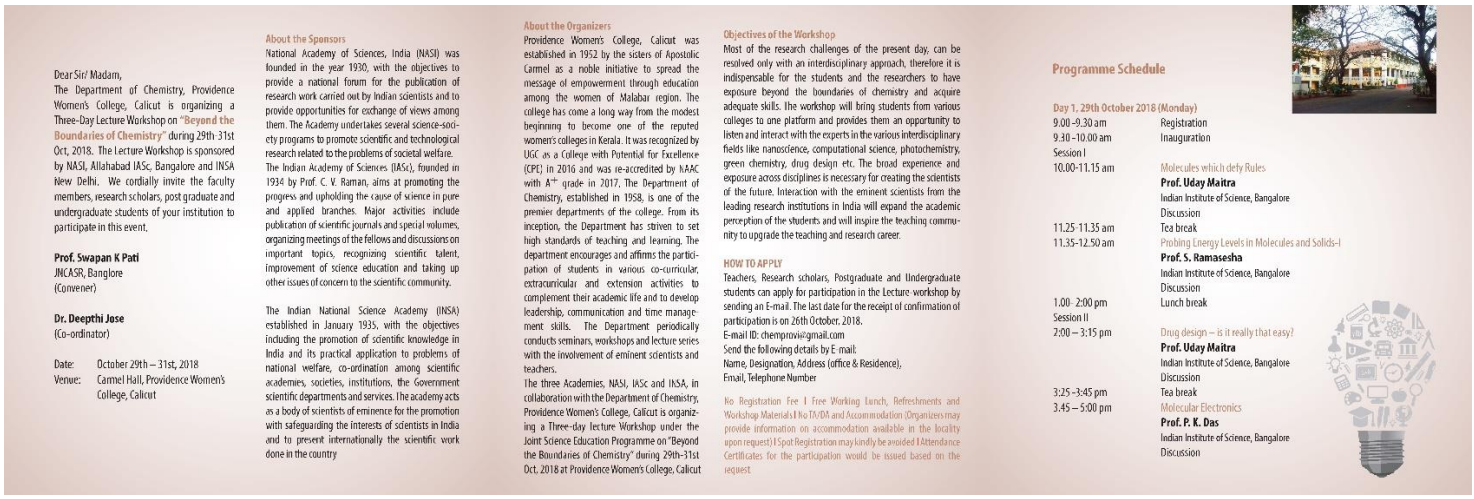
Communications to:
Dr. Deepthi Jose, Asst. Professor, Dept. of Chemistry,
Providence Women's College, Calicut 673009.
Mob: 8547385705

Department of Chemistry
Providence Women's College, Calicut
Tel: 0495 -2371696 Fax: 0495 -2371314
providencecollegecalicut@gmail.com

Sponsored by
The National Academy of Sciences Allahabad
Indian Academy of Sciences Bangalore
Indian National Science Academy New Delhi

Hosted by
Department of Chemistry
Providence Women's College
Calicut, Kerala

SCIENCE ACADEMIES' LECTURE WORKSHOP on
BEYOND THE BOUNDARIES OF
CHEMISTRY
October 29th – 31st, 2018
Providence Women's College, Calicut



Dear Sir/ Madam,

The Department of Chemistry, Providence Women's College, Calicut is organizing a Three-Day Lecture Workshop on "Beyond the Boundaries of Chemistry" during 29th-31st Oct, 2018. The Lecture Workshop is sponsored by NASI, Allahabad IASc, Bangalore and INSA New Delhi. We cordially invite the faculty members, research scholars, post graduate and undergraduate students of your institution to participate in this event.

Prof. Swapan K Pati
JNCASR, Banglore
(Convener)

Dr. Deepthi Jose
(Co-ordinator)

Date: October 29th – 31st, 2018
Venue: Carmel Hall, Providence Women's College, Calicut

About the Sponsors

National Academy of Sciences, India (NASI) was founded in the year 1930, with the objectives to provide a national forum for the publication of research work carried out by Indian scientists and to provide opportunities for exchange of views among them. The Academy undertakes several science-society programs to promote scientific and technological research related to the problems of societal welfare.

The Indian Academy of Sciences (IASc), founded in 1934 by Prof. C. V. Raman, aims at promoting the progress and upholding the cause of science in pure and applied branches. Major activities include publication of scientific journals and special volumes, organizing meetings of the fellows and discussions on important topics, recognizing scientific talent, improvement of science education and taking up other issues of concern to the scientific community.

The Indian National Science Academy (INSA) established in January 1935, with the objectives including the promotion of scientific knowledge in India and its practical application to problems of national welfare, co-ordination among scientific academies, societies, institutions, the Government scientific departments and services. The academy acts as a body of scientists of eminence for the promotion with safeguarding the interests of scientists in India and to present internationally the scientific work done in the country

About the Organizers

Providence Women's College, Calicut was established in 1952 by the sisters of Apostolic Carmel as a noble initiative to spread the message of empowerment through education among the women of Malabar region. The college has come a long way from the modest beginning to become one of the reputed women's colleges in Kerala. It was recognized by UGC as a College with Potential for Excellence (CPE) in 2016 and was re-accredited by NAAC with A^{++} grade in 2017. The Department of Chemistry, established in 1958, is one of the premier departments of the college. From its inception, the Department has striven to set high standards of teaching and learning. The department encourages and affirms the participation of students in various co-curricular, extracurricular and extension activities to complement their academic life and to develop leadership, communication and time management skills. The Department periodically conducts seminars, workshops and lecture series with the involvement of eminent scientists and teachers.

The three Academies, NASI, IASc and INSA, in collaboration with the Department of Chemistry, Providence Women's College, Calicut is organizing a Three-day lecture Workshop under the Joint Science Education Programme on "Beyond the Boundaries of Chemistry" during 29th-31st Oct. 2018 at Providence Women's College, Calicut

Objectives of the Workshop

Most of the research challenges of the present day, can be resolved only with an interdisciplinary approach, therefore it is indispensable for the students and the researchers to have exposure beyond the boundaries of chemistry and acquire adequate skills. The workshop will bring students from various colleges to one platform and provides them an opportunity to listen and interact with the experts in the various interdisciplinary fields like nanoscience, computational science, photochemistry, green chemistry, drug design etc. The broad experience and exposure across disciplines is necessary for creating the scientists of the future. Interaction with the eminent scientists from the leading research institutions in India will expand the academic perception of the students and will inspire the teaching community to upgrade the teaching and research career.

HOW TO APPLY

Teachers, Research scholars, Postgraduate and Undergraduate students can apply for participation in the Lecture workshop by sending an E-mail. The last date for the receipt of confirmation of participation is on 26th October, 2018.
E-mail ID: chemprovi@gmail.com
Send the following details by E-mail:
Name, Designation, Address (office & Residence),
Email, Telephone Number

No Registration Fee I Free Working Lunch, Refreshments and Workshop Materials I No TA/DA and Accommodation (Organizers may provide information on accommodation available in the locality upon request) I Spot Registration may kindly be avoided I Attendance Certificates for the participation would be issued based on the request

Programme Schedule

Day 1, 29th October 2018 (Monday)

9.00 -9.30 am — Registration
9.30 -10.00 am — Inauguration

Session I

10.00-11.15 am — Molecules which defy Rules
Prof. Uday Maitra
Indian Institute of Science, Bangalore
Discussion

11.25-11.35 am — Tea break

11.35-12.50 am — Probing Energy Levels in Molecules and Solids-I
Prof. S. Ramasesha
Indian Institute of Science, Bangalore
Discussion

1.00 -2:00 pm — Lunch break

Session II

2:00 – 3:15 pm — Drug design – is it really that easy?
Prof. Uday Maitra
Indian Institute of Science, Bangalore
Discussion

3:25 -3:45 pm — Tea break

3.45 – 5:00 pm — Molecular Electronics
Prof. P. K. Das
Indian Institute of Science, Bangalore
Discussion

Workshop Banners

Programme Schedule

Programme Schedule

Day 1, 29th October 2018 (Monday)

9.00 -9.30 am	Registration
9.30 -10.00am	Inaugural Session
Prayer	
Welcome	**Dr.Gigy Abraham,** Head, Department of Chemistry
Presidential Address	**Dr. Minoo Divakaran,** IQAC Co-ordinator, Providence Women's College
Keynote Address	**Prof. Swapan K Pati**
	Theoretical Sciences Unit, JNCASR, Bangalore
Vote of Thanks	**Dr.DeepthiJose,** Co-ordinator

Session I 10.00-11.15am

Molecules which defy Rules;
Prof. Uday Maitra, IISc Bangalore

At the UG and PG levels a number of principles are taught in a somewhat general manner. These include principles of stereochemistry, aromaticity, reaction mechanism, reactive intermediates etc. It is important to realize that while these principles generally apply to a large number of molecules and reactions, there are many which do not 'obey' the rules or the principles. This lecture will highlight a number of such principles with molecules which seem to 'defy' such rules and principles!

Discussion

11.25-11.35 am Tea break

11.35-12.50am **Probing Energy Levels in Molecules and Solids-I;**
Prof. S. Ramasesha, IISc Bangalore

Discussion

1.00- 2:00 pm Lunch break

Session II 2:00 – 3:15 pm

Drug Design – is it really that easy?
Prof. Uday Maitra

Despite the availability of useful medicines for many diseases, appropriate drugs are still not available for many others. Drug design is a very complex process which is often misunderstood by many. In this lecture some general principles on drug design will be discussed, followed by highlighting a few examples of common drugs which act through the inhibition of enzymes. Some recently discovered enzyme-inhibiting drugs will also be discussed in the lecture.

Discussion

3:25 -3:45 pm Tea break

3.45 – 5:00 pm **Molecular Electronics;**
Prof. P. K. Das, IISc Bangalore

The first suggestion of using a (organic) molecule as a molecular rectifier was theoretical and came in 1974. Since then molecular electronics have been thought about in the context of miniaturization of electronic circuits and find molecules to provide electronic functions. Nonlinear optical molecules can also serve various applications in molecular electronics in terms of electro-optic switching, all optical switching for data communication and transmission, soliton logic gates and all-optical devices. At the molecular level, it is an organic or inorganic molecule which shows such properties to act as a molecular electronic material. Some of the molecules and methods of optimizing them for the desired properties to have potential application as molecular devices will be presented in this talk

Discussion

DAY 2, 30th October 2018 (Tuesday)
Session III

9.30-10.45 am **Issues of Clean Energy,**
Prof. Sheela K. Ramasesha, NIAS, Bangalore

Energy is an essential part of any society. The way energy is generated to meet the growing demand is detrimental to the society. In India, power generated by coal-fired thermal plants accounts for almost 80% of the power requirement. In addition to power generation these thermal plants give out many greenhouse gases which are responsible for global warming. Green power generation technologies are being developed around the world so that greenhouse gas emissions can be controlled. In the two talks, these green technologies for power generation will be discussed.

Discussion

10.55-11.15 am Tea break

SCIENCE ACADEMIES' LECTURE WORKSHOP on
BEYOND THE BOUNDARIES OF
CHEMISTRY
October 29th – 31st, 2018
Providence Women's College, Calicut

11.15-12.30 pm **Chemical Bonding to Artificial Atoms from Classroom Quantum Theory;**
Prof. Swapan K Pati, JNCASR Bangalore

Chemical bonding to artificial atoms from classroom quantum theory: I shall discuss light waves and light particles; atoms, atomic orbitals, their shape and hybridization; details on Chemical bonding, Molecular Orbital theory and hyper-conjugation; circular quantum dots and how to explain their energy level structure from textbook 2-dimensional simple harmonic oscillator energy level features and their correspondence with atoms and atomic orbitals.

Discussion

12.40- 2.00 pm Lunch break

Session IV

2:00 – 3:15 pm **Photodissociation Dynamics;**
Prof. P. K. Das

Bond breaking and bond making have been the central interest of chemists from the beginning. The most accurate and precise way of breaking a bond is by shining light on a molecule where it absorbs and ascertain that the light energy is sufficient to break a bond. The process of understanding the rate of bond breaking and the underlying mechanism is what is studied in photodissociation dynamics. Since it's half of a chemical reaction which involves both bond breaking and making, photodissociation is also known as "half-reaction". In this seminar I will present the main considerations of photodissociation dynamics taking the example of methyl iodide which has been studied in great detail over the past 60 years with a variety of methods and schemes to understand the C-I bond breaking and its mechanism. Once there were hardly any scientists who were working in the area of chemical dynamics, did not work on methyl iodide. We will look at photodissociation dynamics in general through the developments in methyl iodide dissociation in the ultraviolet.

Discussion

3:25 -3: 35 Tea break

3.35-4.50 pm **Modeling I-V Characteristics of Molecular Systems**
Prof. Swapan K Pati

Modeling I-V characteristics of Molecular systems: In this, I shall discuss some of the fundamental features of doing electronics with molecules, how resistivity, conductivity definition change when one deals with single electron tunneling current, how molecules act as tunneling carrier for electron, a celebrated formalism outlined by Landauer in 1959; quantization of current and how to obtain I-V characteristics of a single level molecule to multi-level complex molecular systems, where Coulomb staircase, Negative differential Conductance and Rectification can be observed and rationalized through modeling.

Discussion

DAY 3, 31st October 2018 (Wednesday)
Session V

9.30-10.45 am **Probing Energy Levels in Molecules and Solids II**
Prof. S. Ramasesha

Discussion

10.55-11.15 am Tea break

11.15-12.30 pm Computational Methods

Computational Methods: Quantum Chemistry and wave mechanics, Schrodinger equation and how to solve it. Various approaches, wave function based and Hamiltonian based methods. Hartree-Fock to Configuration Interaction, MP perturbation, Coupled Cluster and CASSCF methods. Density Functional Theory and Semi-empirical methods like Huckel, Hubbard, PPP, CNDO, INDO, AM1 and a few others.

Prof. Raghu C.;NIT Calicut
Prof. Swapan K Pati , JNCASR Banglore

Discussion

12.40 – 2:00 pm Lunch break

Session VI

2.00- 3:15 pm **Green Energy Technologies**
Prof. Sheela K. Ramasesha

Discussion

3.25-3.35 Tea break

3.35-4.50 pm **Challenges in Computational Chemistry**

Challenges in Computational Chemistry: I shall weigh and compare wave function based and Hamiltonian based methods by considering several molecular to solid systems. The set current methods which exist and people use and what they lack and generation of newer methods will be discussed.

Prof. Raghu C.; Prof. Swapan K Pati

5.00 – 5.15 pm Valedictory Session

Photo Gallery

Our Eminent Resource Persons

Participants

Dr. Gigy Abraham, H.O.D, welcoming the gathering and Dr. Deepthi Jose, Coordinator expressing vote of thanks.

Group Photo