Report of the Science Academies' Lecture– Workshop on

Recent Developments in Physical Chemistry

The lecture Workshop on Recent Developments in Physical chemistry sponsored by the three academies, Indian Academy of Sciences, Indian National Science Academy and the National Academy of Sciences, India, was organised at St. Joseph's College, Irinjalakuda, Kerala on 31st January and 1st February 2014. There were 143 participants 35 teachers and 108 students from nearby colleges. The workshop was intended to give an insight to students and teachers about the frontier areas of research in the field of Physical Chemistry with special thrust on Computational Chemistry. The objective of the workshop was to bring students from various colleges to one platform for discussing and presenting the recent developments in Physical Chemistry. It provided an opportunity for them to interact, share and exchange their experiences with resource persons. Well experienced resource persons like Prof. E D Jemmis and Prof. M S Gopinathan could motivate and induce research aptitude in the participants particularly in the field of Computational Chemistry.

The inaugural function scheduled at 9-15 A M was cancelled due to the unexpected demise of one of our faculty members, Ms. Sheena P C, Assistant Professor, department of English, St. Joseph's College. The college was paying the final homage to the departed soul at 9-30 AM in the college auditorium.

The workshop started at 10 AM with the lecture on Nobel laureates in Chemistry 2013 by Prof. M S Gopinathan from IISER, Thiruvanantahapuram. Martin Karplus, Michael Levitt and Arieh Warshel were awarded the Nobel Prize in Chemistry in 2013. In the 1970s, Martin Karplus, Michael Levitt and Arieh Warshel laid the foundation for the powerful programs that are used to understand and predict chemical processes. The strength of the methods that Karplus, Levitt and Warshel have developed is that they are universal. They can be used to study all kinds of chemistry; from the molecules of life to industrial chemical processes. Experts say the work of Karplus, Levitt and Warshel is ground-breaking because they managed to make Newton's classical physics work side-by-side with the fundamentally different quantum physics. Previously, chemists had to choose to use either or. The Nobel laureates in chemistry 2013 have made it possible to map the mysterious ways of chemistry by using computers. Detailed knowledge of chemical processes makes it possible to optimize catalysts, drugs and solar cells.

After a short tea-break the next class started at 11-30 AM by Prof. R S Swathi from IISER, Thiruvananthapuram. Her lecture was on 'Insights into some exactly solvable problems in Quantum Mechanics'. She started with the solution of Schrodinger equation for a particle in a box and explained how the imaginary problem of particle in a two dimensional box is used to study real molecules like benzene. The participants were really excited to find such applications which they had not been aware of during their study of Quantum Chemistry.

The lunch break was shortened by 15 minutes and the next lecture started at 1-45 PM itself. Prof. E G Jayasree, from Kerala University (she was a student of St. Joseph's) gave an introduction of semi-empirical and ab initio methods. Semi-empirical methods use parameters derived from experimental data to simplify the computation. They solve an

approximate form of the Schrodinger equation that depends on having appropriate parameters available for the type of chemical system under investigation. Ab initio methods use no experimental parameters in their computations. Instead, their computations are based solely on the laws of quantum mechanics and on the values of a small number of physical constants.

We had the last lecture of the day by Prof. E D Jemmis, the convener of the workshop. His lecture was on 'Chemistry with Computers'. The fact that scientists these days can use computers to carry out experiments has yielded a much deeper understanding of how chemical processes play out. Computer models mirroring real life have become crucial for most advances made in chemistry today. Chemists earlier used to create models of molecules using plastic balls and sticks. Now, the modelling is carried out in computers. Today the computer is just as important a tool for chemists as the test tube. Simulations are so realistic that they predict the outcome of traditional experiments. Scientists can optimize solar cells, catalysts in motor vehicles or even drugs, to take but a few examples.

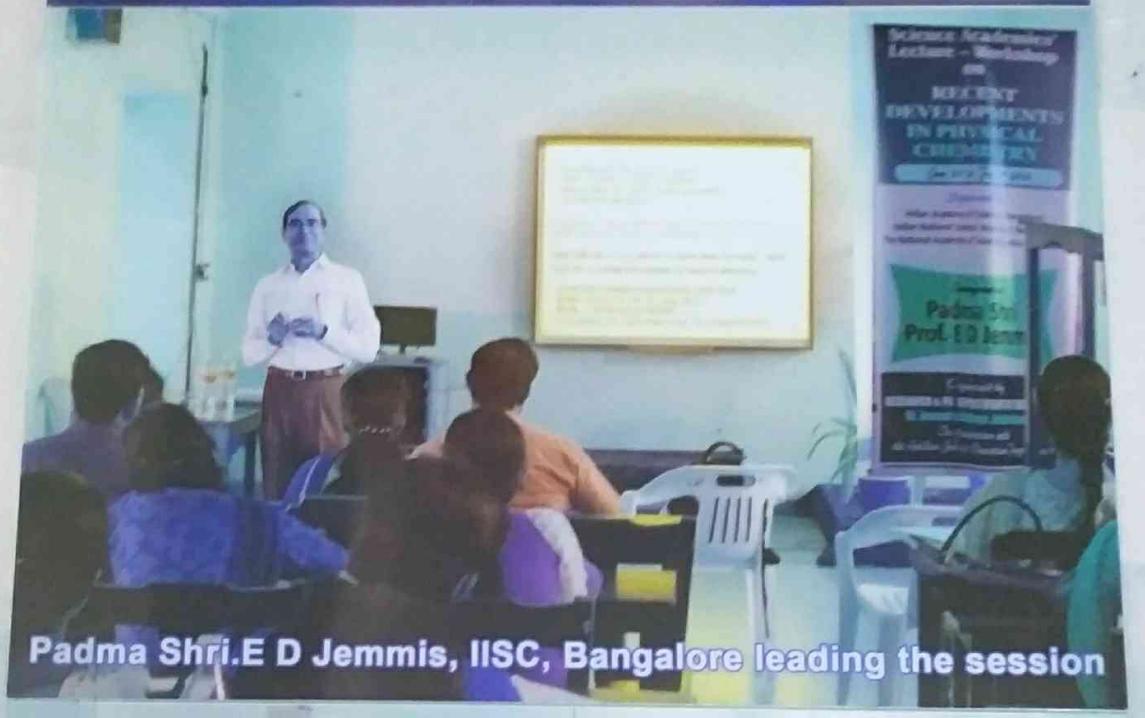
The second day's programme started at 9-15 AM with the first lecture by Prof. M S Gopinathan on Density Functional Theory. Density functional theory (DFT) is a quantum mechanical modelling method used in physics and chemistry to investigate the electronic structure(principally the ground state) of many-body systems, in particular atoms, molecules, and the condensed phases. With this theory, the properties of a many-electron system can be determined by using functionals, i.e. functions of another function, which in this case is the spatially dependent electron density. Hence the name density functional theory comes from the use of functionals of the electron density. DFT is among the most popular and versatile methods available in condensed-matter physics, computational physics, and computational chemistry.

Next session was by Prof. Swathi in which she continued her lecture on 'Insights into some exactly solvable problems in Quantum mechanics'. She showed how Schrodinger equation can be solved to explain the bonding in H_2^+ molecule. The method can be extended to study molecules with more number of electrons but only with certain approximations.

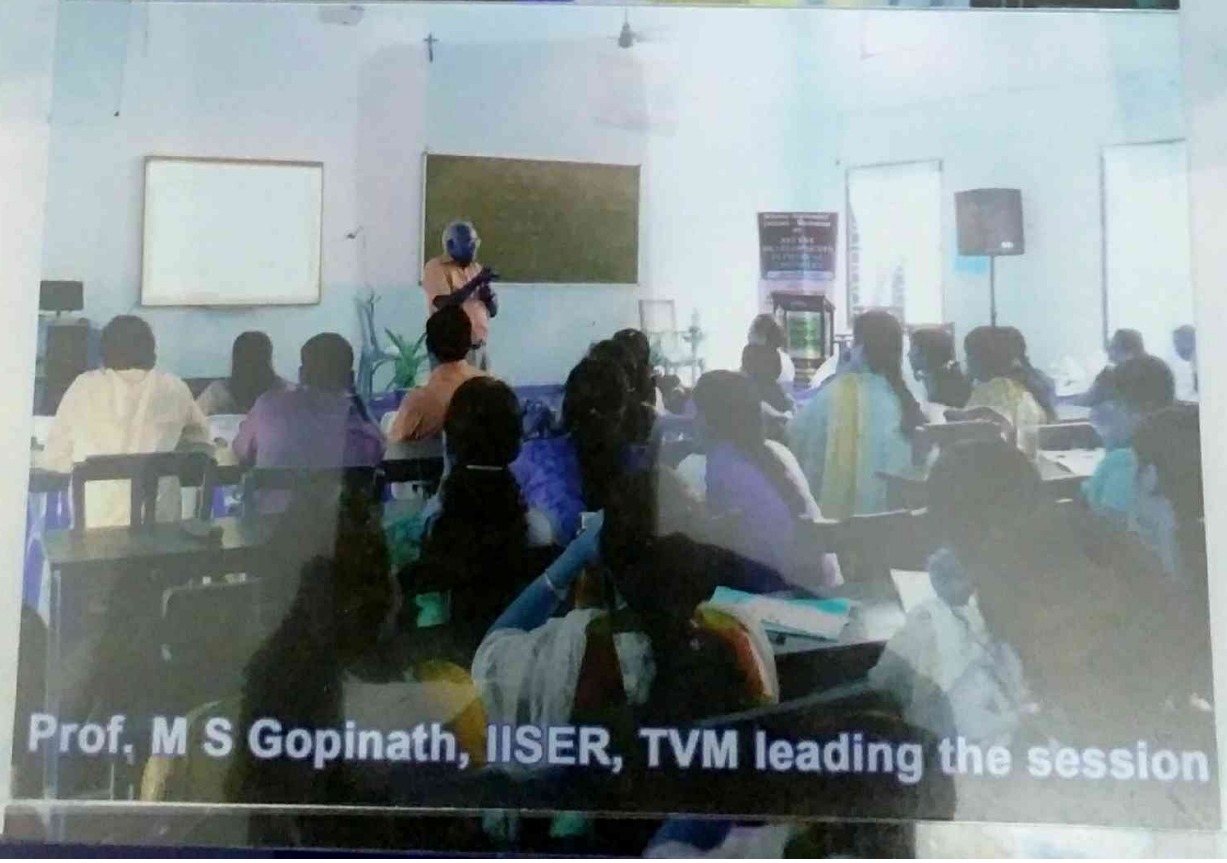
After the lunch Prof. Jemmis delivered the lecture on Problems in Computational Chemistry. Taking H_3 as example he showed how to use principles of Quantum Mechanics and Symmetry to study the properties of molecules. He discussed the techniques for modelling reactions, how to compute activation energies and to determine transition state structure.

The last lecture was by Prof. Jayasree on Molecular Mechanics and Force Fields. Molecular mechanics uses classical mechanics to model molecular systems. The potential energy of all systems in molecular mechanics is calculated using force fields. Molecular mechanics can be used to study small molecules as well as large biological systems or material assemblies with many thousands to millions of atoms. In molecular mechanics, each atom is simulated as a single particle; each particle is assigned a radius (typically the van der Waals radius), polarizability, and a constant net charge (generally derived from quantum calculations and/or experiment). Bonded interactions are treated as "springs" with an equilibrium distance equal to the experimental or calculated bond length. Variations on this theme are possible; for example, many simulations have historically used a "united-atom" representation in which each terminal methyl group or intermediate methylene unit was considered a single particle, and large protein systems are commonly simulated using a "bead" model that assigns two to four particles per amino acid.

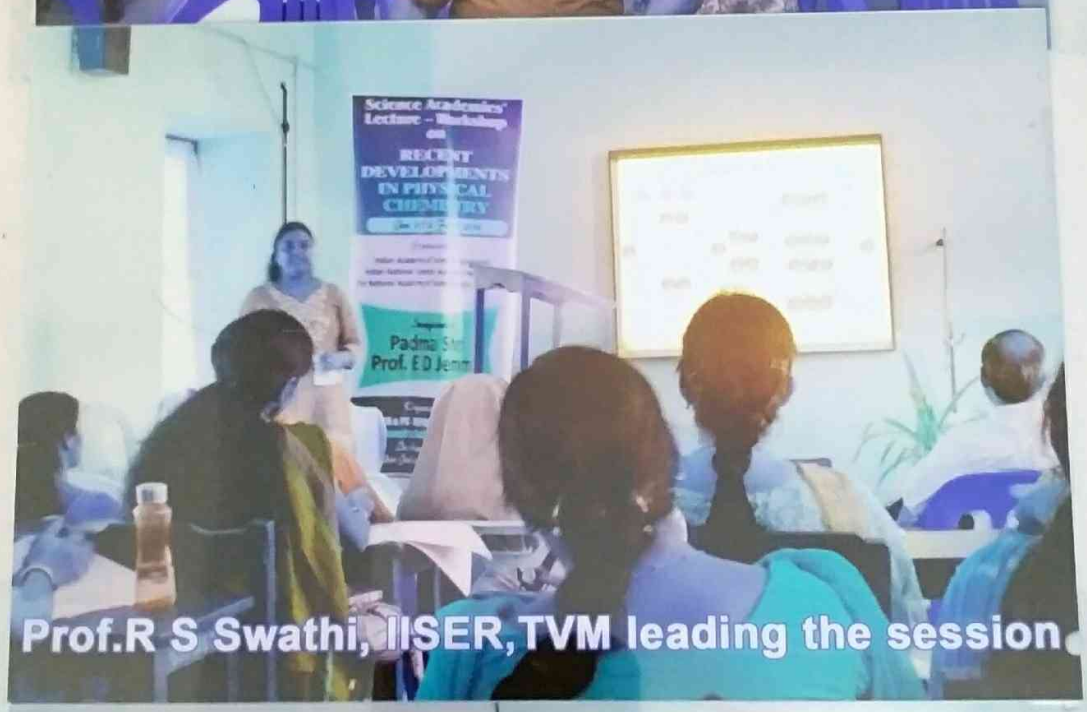
The valedictory session started at 4-15 P M which was presided over by our Principal, Dr. Sr. Annie Kuriakose. The participants expressed their views regarding the conduct and content of the programme. Dr. Tom Cherian, Assistant Professor, Christ College, Irinjalakuda, appreciated the topics and presentation of the workshop. All the participants appreciated the hospitality and organisation. Then the Principal felicitated the Padmasree recipient Prof. E D Jemmis and wished him success in his future endeavors to scale new heights in the field of scientific research. Prof. Jemmis emphasised the need of doing research for the progress of India and mankind. Dr. Rosabella K Puthur, the Head of the department of Chemistry and the Coordinator of the workshop proposed the vote of thanks. The programme got over by 4-45 PM



Padma Shri.E D Jemmis, IISC, Bangalore leading the session



Prof. M S Gopinath, IISER, TVM leading the session



Prof.R S Swathi, IISER,TVM leading the session

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