# REPORT OF THE

## Two Day International Seminar

# 'NEW HORIZONS IN CHEMISTRY'

## 5TH & 6TH September 2013

### ORGANIZED BY PG AND RESEARCH DEPARTMENT OF CHEMISTRY, ST. JOSEPH'S COLLEGE , IRINJALAKUDA

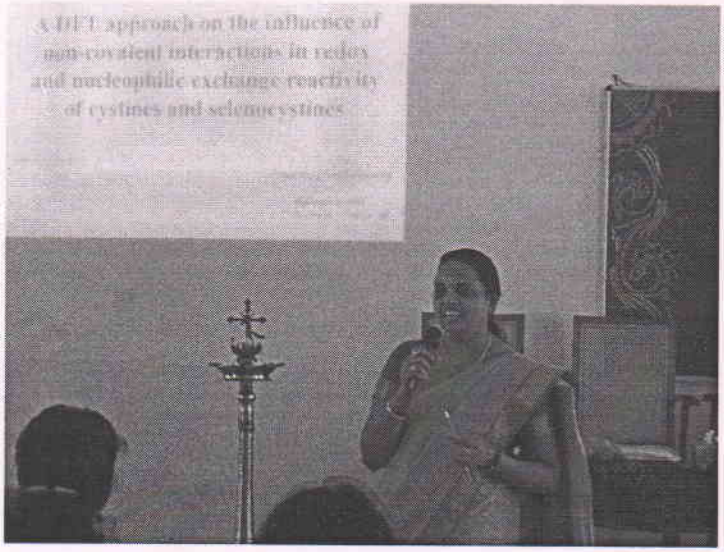
The **Inaugural programme** started at 9.30 am in the Chemistry Hall with Dr. Sr. Annie Kuriakose, Dr. II Mathews, Dr. Rosabella K Puthur and Ms .Mary Augustine on stage. Ms. Rosabella K Puthur offered a warm welcome to the all those who were present for the inaugural function. Dr. Sr. Annie Kuriakose delivered the presidential address in which she stressed the importance of such scientific interactions. She also thanked Ms. Mary Augustine for her sincere service to the institution.

Dr. I I Mathews inaugurated the function followed by his keynote address. In his keynote address, he explained the use of synchotorn in analysis and research of drug materials. After his keynote address Ms. Nisha Nandakumar, Assistant professor, FISAT, Angamaly felicitated her teacher Ms. Mary Augustine. Dr. Binsy Varghese. V, convener of the programme, offered the formal vote of thanks.

After tea break Dr. I I Mathews, Staff Scientist, SLAC, Stanford ,USA, took class on Structure based Drug Design. Structure-based drug design is a powerful method, especially when used as a tool within an armamentarium, for discovering new drug leads against important targets. After a target and a structure of that target are chosen, new leads can be designed from chemical principles or chosen from a subset of small molecules that scored well when docked in silico against the target. After a preliminary assessment of bioavailability, the candidate leads continue in an iterative process of reentering structural determination and reevaluation for optimization. Focused libraries of synthesized compounds based on the structure-based lead can create a very promising lead which can continue to phase I clinical trials. As structural genomics, bioinformatics, and computational power continue to explode with new advances, further successes in structure-based drug

determined at an amazing rate, and our capability to capture a quantitative picture of the interactions between macromolecules and ligands is accelerating. The session was concluded at 12.30.

After Lunch the second session began at 1.30 with Dr. E G Jayasree, Assistant professor, Dept. of Chemistry, Kerala university as the resource person. Her topic was 'A DFT approach on the influence of non-covalent interactions in redox and nucleophilic exchange reactivity of cystines and selenocystines'. 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 atoms, 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, and computational chemistry.



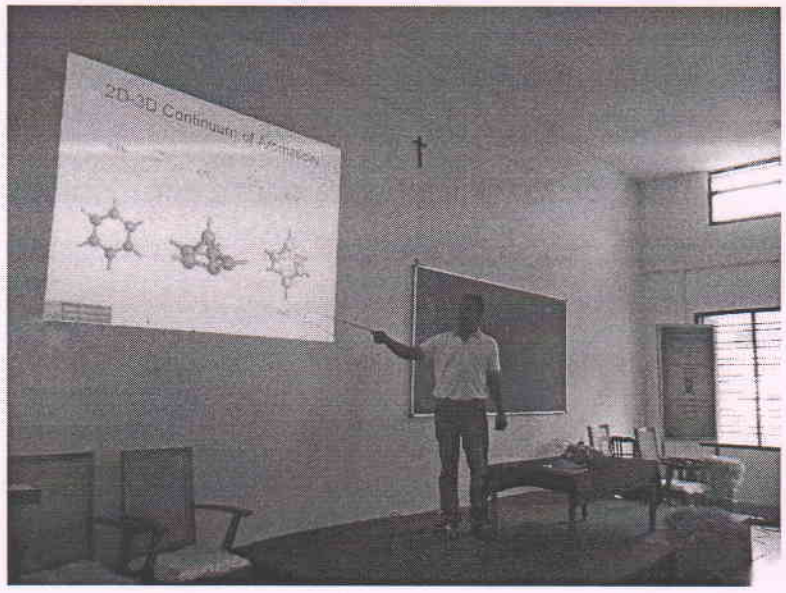

After tea break at 3.45, the last session began. Ms. Nisha Nandakumar, Ms. Mity Thambi, Dr. S .Maya Devi, Dr. Sr Lilly Kachappilly presented their research papers in this session. Dr. Pearly Sebastian, the joint convener of the programme, chaired the session.

On 6th September the first session was engaged by Dr. R S Swathi, IISER, Thiruvananthapuram. She gave an interesting class on 'Graphyne and Graphdyne, new Materials in carbon family'. Carbon nanotubes and graphene have paved the way for the next step in the evolution of carbon materials. Among the novel forms of carbon allotropes is graphyne – a two-dimensional lattice of sp–sp2-hybridized carbon atoms similar to graphene for which recent progress has been made in synthesizing dehydrobenzoannulene precursors that form subunits of graphyne. Atomistic modeling is carried out to determine its mechanical properties for both in-plane and bending deformation including material failure, as well as intersheet adhesion. Unlike graphene, the fracture strain and stress of graphyne depends strongly on the direction of the applied strain and the alignment with carbon triple-bond linkages,

plane bending stiffnesses are comparable to graphene, despite the density of graphyne being only one-half of that of graphene. Unlike graphene, the sparser carbon arrangement in graphyne combined with the directional dependence on the acetylenic groups results in internal stiffening dependent on the direction of applied loading, leading to a nonlinear stress–strain behavior.

After tea break, five paper presentations were done. Ms. Ambily K U, Ms. Aswathy PR, Ms. Indu V R, Ms. Divya C and Ms. Fahima A A presented their research results.

The last session was handled by Dr. M M Balakrishna Rajan, Assistant professor, Dept. of Chemistry, Pondichery University. The topic of the lecture was ' Benzyne analogs of polyhedral boranes, Same but not so same'. An interesting feature of elemental boron and boron compounds is the occurrence



of highly symmetric icosahedral clusters. The rich chemistry of boron is also dominated by three-dimensional cage structures. Despite its proximity to carbon in the periodic table, elemental boron clusters have been scarcely studied experimentally and their structures and chemical bonding have not been fully elucidated. The experimental and theoretical evidence that small boron clusters prefer planar structures and exhibit aromaticity and antiaromaticity according to the Hückel rules, like planar hydrocarbons. Aromatic boron clusters possess more circular shapes whereas antiaromatic boron clusters are elongated, analogous to structural distortions of antiaromatic hydrocarbons. The planar boron clusters are thus the only series of molecules other than the hydrocarbons to exhibit size-dependent aromatic and antiaromatic behaviour and represent a new dimension of boron chemistry. The stable aromatic boron clusters may exhibit similar chemistries to that of benzene, such as forming sandwich-type metal compounds.

After the tea break, there were 11 paper presentations. As it became so late the valedictory function was made short and consisted of only evaluation and a formal vote of thanks by Dr. Pearly Sebastian, the joint convener of the programme.

There were altogether 118 participants out of which 45 were outstation participants. We provide working lunch for two days four sevings of tea also.