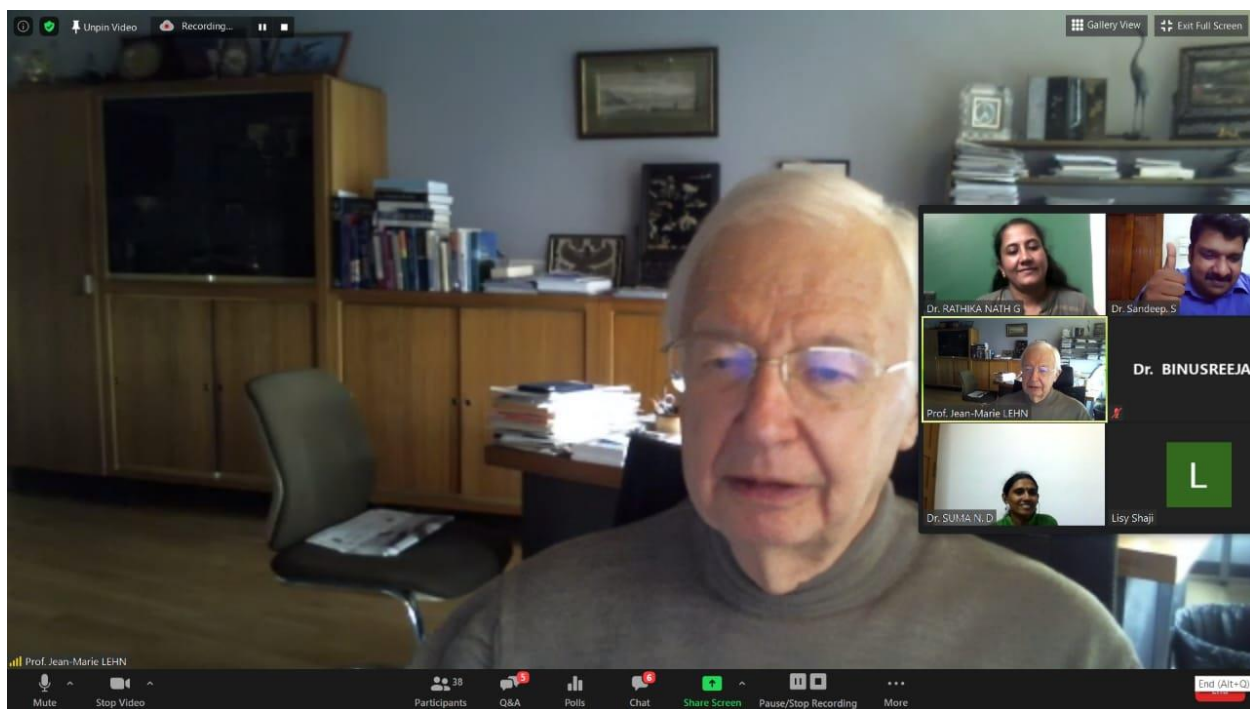


**REPORT ON THE INTERNATIONAL CONFERENCE ON EMERGING
TRENDS IN COMPUTATIONAL AND MATERIALS CHEMISTRY
RESEARCH (ICCMCR-2020)**

Department of Chemistry and Polymer Chemistry organized an international conference from 9th to 12th November 2020 on “**EMERGING TRENDS IN COMPUTATIONAL AND MATERIALS CHEMISTRY RESEARCH**”.

The theme of the conference was the contemporary advances and innovations in computational and material chemistry research. The international conference aimed to provide a forum for researchers from various areas of materials Chemistry, medicinal Chemistry and Computational Chemistry to present their latest cutting-edge research findings and share their experiences and research outcomes of interdisciplinary research. Each session of the conference included expert lectures, paper presentations and discussions on computational and materials chemistry research. Registration was open from 14th October 2020 till 05th November 2020. More than hundred participants got registered via google forms.

The Conference was inaugurated by Prof. Jean-Marie Lehn , Nobel Laureate in Chemistry (1987) on 09th November 2020. He delivered an excellent talk on supramolecular chemistry and it was followed by a hot discussion on the new trends in the computational designing of supramolecules. Around 115 delegates in and out of the State participated in the entire session of his lecture.



DYNAMIC COVALENT CHEMISTRY DCC
 implementing **REVERSIBLE REACTIONS**
AMINE - CARBONYL CONDENSATIONS

Imine Formation

$$A-NH_2 + \begin{array}{c} O \\ \parallel \\ C \\ | \\ X \end{array} B \rightleftharpoons A-N=C \begin{array}{c} B \\ | \\ X \end{array} + H_2O$$

Acylhydrazone Formation

$$A-C(=O)-NH-NH_2 + \begin{array}{c} O \\ \parallel \\ C \\ | \\ X \end{array} B \rightleftharpoons A-C(=O)-NH-N=C \begin{array}{c} B \\ | \\ X \end{array} + H_2O$$

- ✓ organic and biological groups
- ✓ compatible with aqueous phase
- ✓ kinetics controllable by pH

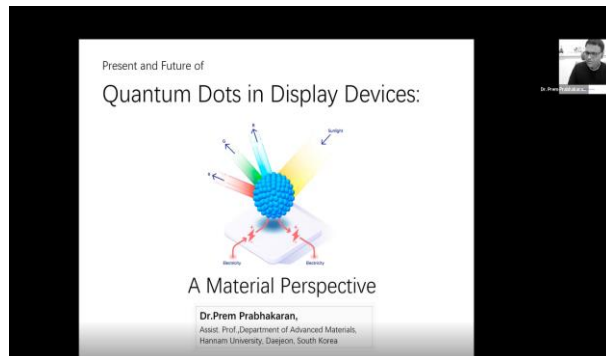
Day 1 : Inaugural talk by Nobel Laurate Prof. Jean-Marie Lehn

On the same day , Dr. Prem Prabhakaran, Department of Advanced Materials, College of Life Science and Nanotechnology Hannam University, South Korea had given a motivational and inspirational talk on present and future of quantum dots. Dr. Prem's session was exciting and had a participation of 68

delegates. The third session was handled by Dr. Cheol Woo Ha , Korea Additive Manufacturing Innovation Center, Korea Institute of industrial Technology, Korea . He had delivered a talk on 3D printing and photon polymerization. Cheol's discussion was about the development of 3D printing in the biomedical field and around 65 delegates actively participated in that lecture session.



DAY 1 , Dr. Cheol Woo Ha



DAY 1 , Dr. Prem Prabhakaran


The second day (10th November) of the international conference started with the lecture of Prof. Dr. Nagaiyan Sekar , Former Head , Department of Dye stuff Technology, Professor in Tinctorial Chemistry Institute of Chemical Technology, Mumbai. He had given a talk on Non-linear optical properties of colorants - a computational approach. Second session was handled by Dr. G.Gopakumar, Fuel Chemistry Division, IGCAR, Kalpakkam. He had given the talk on ‘Computational Chemistry of Lanthanide and actinide metal complexes.’




**Computational Studies on
Actinide Metal Complexes**

Dr. G. Gopakumar
Indira Gandhi Centre for Atomic Research
Kalpakkam, 603 102 Tamil Nadu
India
10 November 2020

Day 2



Non-Linear Optical Properties of Colorants - Computational Approach
Nonlinear optics deals with phenomena arising from light induced changes in the optical properties of materials.
The interaction of light with a nonlinear optical (NLO) material gives rise to new optical fields with altered properties (e.g., phase, frequency, amplitude, polarization, path, etc.)
several NLO effects had been proposed or demonstrated beforehand
M. Goepfert-Mayer, Ann. Phys. 9 (1931) 273
Following demonstration of the first working laser
A.L. Schawlow, C.H. Townes, Phys. Rev. 112 (1958) 1940.
T.H. Maiman, Nature 187 (1960) 493.
Materials with significant NLO properties have various technological applications such as
data storage,
optical computing,
optical communication,
optical switches,
frequency generation, etc.

International Conference on Emerging Trends in Computational
and Materials Chemistry Research from 8 to 12 November
2020



Day 2, Prof. Dr. Nagaiyan Sekar

Day 3 , Dr. Vineeth Vijayan

Afternoon was the time for presentations . About fourteen participants comprising Students , Research scholars & Teachers in and out of our College / State presented papers in various research topics. Dr.Vineeth Vijayan , Department of Material Science and Engineering Centre for Nanoscale Materials and Biointegration University of Alabama Birmingham ,United Staes had given us a talk on the topic ‘ Polymeric biomaterials and Plasma surface modifications’ in the evening of the second day.

The first session of the third day of the international conference (11 th November) was handled by Dr.Viola.B.Morris, Division of Cardiology, Emory University School of Medicine, Atlanta . The session had an enthusiastic talk on Arginine functionality for delivery of therapeutics. Around 64 delegates attended her talk. The second session on the same day was of Dr. Bartolome Soberats, Ramony Cajal Research Fellow Dept. of Chemistry, Universitat de les Illes Balears, Spain. His lecture was on ‘liquid crystalline materials’ and around 52 delegates participated in that session . Later from 3 pm onwards it was the time for presentations . Students , Research scholars & Teachers presented papers in various research topics.

L-Arginine therapy in cardiovascular pathologies: beneficial or dangerous?
 Rainer H. Böger
 Current Opinion in Clinical Nutrition and Metabolic Care 2008, 11:55-61

+ L-arginine? PLUS.
 Adding L-arginine to your diet increases Nitric Oxide production in your body.

Nitric Oxide Energy
 Boosts Nitric Oxide and increases Blood Flow

Healthy Artery

The Nobel Prize landmark discovery of the functions of Nitric-Oxide (NO) as a signaling molecule showed that Nitric-Oxide helps cardiovascular walls relax with each heartbeat to enable arterial expansion and contraction.

R.H. Böger et al. Circulation 1997

Day 3 Dr.Viola.B.Morris,

supramol UIB soberats Characterization of Liquid Crystals

Polarizing Optical Microscopy

Differential Scanning Calorimetry

X-Ray

10

Day 3 Dr. Bartolome Soberats

On the final day of the International Conference, Nov 12th, Prof. Dr. Edamana Prasad, Department of Chemistry, IIT, Madras was the first resource person to deliver the talk. His topic was about the ‘Light emitting Gels and their applications’. Prof. Dr. Johannes Gierschner, IMDEA Nanoscience, Madrid, Spain in the afternoon session, discussed photo catalysis as well as photo physics. He demonstrated the computational designing in organic photo catalysis. Around 55 delegates participated in that photocatalysis session. Dr. Pradeep P. N. Syamala Department of Chemistry, University of Wuerzburg, Germany handled the evening session and the topic was again Supramolecular Chemistry : From Molecules to Functional Materials.



Day 4, Dr Pradeep P N Syamala



Day 4 Dr Edamana Prasad

Home / People / Researchers / Gierschner

Prof. Johannes Gierschner



Position: Senior Research Prof.
PhD: University of Tübingen, Germany
Previous Position: University of Mons, Belgium
Research: Photophysics of Organic and Hybrid Supramolecular Nanosystems
ORCID: 0000-0001-8177-7919
Researcher ID: K-7938-2014

Day 4



Day 4 Valedictory Function , Dr Sabu Thomas

More than hundred and fifty delegates participated in the entire sessions of the Conference. Mode of the event was Google meet and YouTube . In the Valedictory Session on Nov 12th at 7.00 pm, Prof. Dr. Sabu Thomas Hon. Vice Chancellor, M.G University , Kottayam, Kerala chaired the meeting. After delivering the valedictory speech he announced the best paper award for Smt.Rekha Koshy, Assistant Professor , Bishop Moore College, Mavelikkara . Her presentation was on the topic carbon dots and chitin nanowhisker in food packaging.The meeting came to an end at 8.00pm.

