

**National seminar on "Industrial Advances in Green Chemistry and Sustainability" Organized by the Department of Chemistry, St. Joseph's College (Autonomous), Irinjalakuda on 6<sup>th</sup> & 7<sup>th</sup> February 2020**

The Department of Chemistry, St. Joseph's College (Autonomous), Irinjalakuda organized two day national seminar on Industrial Advances in Green Chemistry and Sustainability on 6<sup>th</sup> & 7<sup>th</sup> February 2020. The seminar was inaugurated by Dr. Kumar V, Senior Scientist, C-MET, Thrissur. More than hundred delegates from various colleges and Research centres were participated in the seminar. Dr. Deena Antony C, Head of the Department of Chemistry welcomed the gathering. Dr. Sr. Lissy Anto P, Principal, St. Joseph's College (Autonomous), Irinjalakuda delivered the presidential address. The convenor of the seminar Ms. Vidhya Thomas K proposed the vote of thanks. Dr. Kumar V, Scientist, C-MET, Thrissur, Dr. Abdul Khayum Mohammed, Research Associate, IISER Kolkata, Dr. Ranjith S Pillai, Assistant Professor, SRM Institute of Science and Technology, Chennai and Dr. Pradeepan Periyat, Assistant Professor, University of Calicut, were the resource persons of the seminar.

The keynote lecture was delivered by Dr. Kumar V on Chemistry of materials. In his talk he explained the need to design and develop new materials. Demands are diverse. While there is a need to design and develop new materials there is also an ever increasing demand to develop appropriate synthetic protocols for materials in nanosize as well as with exquisite architectures. Structure-property correlation of materials is also gaining importance as we strive to understand the root-cause of materials characteristics to exploit them in many ways. Chemistry not only provides insights into the above but also promises exciting solutions to the diverse requirements. These will be highlighted in the lecture.

Dr. Abdul Khayum Mohammed, Research Associate, IISER Kolkata, delivered lecture on Covalent organic frameworks for energy storage and water purification. He stated that the research on porous materials gain increasing attention due to their potential properties in various fields like gas storage; catalysis; energy storage; sensors; drug-delivery; opto-electronics etc. He explained that the covalent organic frameworks can be served as excellent energy storage materials due to the ordered intrinsic micro or mesoporous structure with redox-active backbone and the high surface area. Whereas, these advantages are absent in the conventional amorphous carbon based materials or polymers used for the energy storage applications. He discussed 2 types of charge storage mechanisms 1) electric double layer capacitance (EDLC) 2) surface redox capacitance. He also added that the software controlled three dimensional (3D)

macro-architecture of functional porous materials gains tremendous scientific and technological attention towards the molecular uptake.

Paper presentations by the selected participants were arranged in the afternoon session.

On the second day of the national seminar, the keynote lecture was delivered by Dr. Pradeepan Periyat, Assistant Professor, University of Calicut, on Infrared reflective inorganic pigments. An inorganic pigment means a substance which consists of small particles that are practically insoluble in any of the solvents and binders. The color produced by inorganic pigments is a sense-impression evoked by rays of light entering the eye. If the light source itself is standardized, the optical properties of a pigmented layer of paint depend on the optical properties of the pigment particles, their size, shape, and volume concentration, and also on the optical properties of (usually colorless) dispersion medium. In this talk, history of pigments, its classification are discussed and later focus on recent developments of the near infrared reflecting inorganic pigments. The aim of this talk is to classify these pigments based on their color, to explain synthesis methods and to discuss the optical properties.

Next lecture was continued by Dr. Pradeepan Periyat on the optical properties of inorganic pigments. The multifunctional inorganic pigments absorb the visible region of the solar spectrum and reflect the NIR portion. Recent trends in the optical properties of NIR reflecting inorganic pigments published in literature make the scientific community to design and develop "Cool pigments" for surface coating applications, coloration of plastics and ceramics. The cool roofs can reduce the heat build-up inside the building and this makes unconditioned building more comfortable and decrease the amount of cooling power in conditioned buildings. Inorganic pigments also contribute to the enjoyment, beauty and functionality of the objects bring into the world. To ensure that their benefits far outweigh their liabilities, research efforts are directed towards the development of environmentally acceptable pigments those do not release any toxic materials into the environment during their production, use and disposal.

Dr. Ranjith S Pillai, Assistant Professor, SRM Institute of Science and Technology, Chennai was the resource person in the last session on the topic Computational design of porous solids for industrial relevant gas storage and separations. Dr. Ranjith described on a synergistic experimental/modeling approach to design novel porous solids with optimal separation performances for diverse binary and ternary mixtures of interest including  $\text{CH}_4/\text{N}_2$ ,  $\text{N}_2/\text{O}_2$ ,  $\text{CH}_4/\text{H}_2\text{O}$ ,  $\text{CH}_4/\text{CO}_2$ ,  $\text{CH}_4/\text{CO}_2/\text{H}_2\text{O}$ ,  $\text{CH}_4/\text{CO}_2/\text{H}_2\text{S}$  and further unveil the microscopic origin of the separation mechanisms in play. The computational effort integrated a subtle combination of

Density Functional Theory (DFT) calculations, derivation of specific force field and Grand Canonical Monte Carlo (GCMC) simulations. He also discussed about a fluorinated small pore MOF containing open metal sites, namely the AlFFIVEH<sub>2</sub>O-1-Ni with unique separation performances for CH<sub>4</sub>/CO<sub>2</sub>/H<sub>2</sub>O, CH<sub>4</sub>/CO<sub>2</sub>/H<sub>2</sub>S. DFT simulations demonstrated that this solid can concomitantly adsorb CO<sub>2</sub> and either H<sub>2</sub>O or H<sub>2</sub>S which makes AlFFIVEH<sub>2</sub>O-1-Ni as a unique adsorbent to simultaneously dehydrate and purify CH<sub>4</sub>. He also extended his talk about an unprecedented capture of N<sub>2</sub> for both natural gas upgrading and air separation using a mesoporous Metal-Organic Framework material containing accessible Cr(III) sites. A combination of advanced experimental and computational tools revealed that the separation mechanism for both N<sub>2</sub>/CH<sub>4</sub> and N<sub>2</sub>/O<sub>2</sub> gas mixtures is driven by the presence of these unsaturated Cr(III) that allows a much stronger binding of N<sub>2</sub> vs CH<sub>4</sub> and O<sub>2</sub>. This concept opens new horizons to address several challenges in chemistry, such as the removal of nitrogen or the design of heterogeneous biomimetic catalysts through nitrogen fixation.

Most of the participants are interacted with the invited speakers and enjoyed the lectures. Dr. Manoj A L delivered the valedictory address. In his speech he stressed the importance of Science and Research and also role of Chemist in the present and future Scenario.