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Notice for the PhD Viva Voce Examination

Mr Muthukumar D, Registration Number: 2170239, PhD Scholar at the Department of Chemistry, School of Sciences, CHRIST (Deemed to be University) will defend his PhD thesis at the public viva-voce examination on Wednesday, 04 June 2025 at 11.30 am in Room No. 044, Ground Floor, R & D Block, CHRIST (Deemed to be University), Bengaluru - 560029, Karnataka, India.

Title of the Thesis	:	**Designing Porous Materials for Capture and Utilization of Toxic Gases Expelled from Power Plants with Molecular Modelling Techniques**
Discipline	:	**Chemistry**
External Examiner - I	:	**Dr Kuntal Manna** Associate Professor Department of Chemistry Indian Institute of Technology Delhi Hauz Khas, Delhi - 110016 New Delhi
External Examiner – II	:	**Dr P S Mukherjee** Professor Inorganic and Physical Chemistry Department Indian Institute of Science Bengaluru - 560029 Karnataka
Supervisor	:	**Dr Sunaja Devi K R** Professor Department of Chemistry School of Sciences CHRIST (Deemed to be University) Bengaluru - 560029 Karnataka

The members of the Research Advisory Committee of the Scholar, the faculty members of the Department and the School, interested experts and research scholars of all the branches of research are cordially invited to attend this open viva-voce examination.

Registrar (Academics)

Place: Bengaluru
Date: 02 June 2025

ABSTRACT

The high energy demand for population growth leads to the development of industries worldwide, especially coal-fired power plants, which are one of the main causes of the emission of toxic gases. The entire globe is witnessing the potential influence of climatic change and global warming due to man-made emissions of various gases such as CO2, SO2, and NO2 which remain on an upward trend. To mitigate the toxic gas emission, adsorption and utilizing the adsorbed toxic gases as a value-added chemical is one of the cheaply available techniques, and it is identified as a convenient technology for industrial plants. Metal Organic Frameworks (MOFs) are found to be the predominant porous material for the toxic gas adsorption and utilization due to their versatile properties.

The ultimate goal of this thesis is to develop new porous materials using molecular modelling techniques for the adsorption of toxic gases such as CO2, SO2, and NO2 and utilizing them into value-added chemicals such as cyclic carbonates, sulphites, and nitrates, respectively, using computational simulations. Density Functional Theory (DFT) and the Grand Canonical Monte Carlo (GCMC) simulations are the crucial methodologies for the toxic gas adsorption and Climbing Image Nudged Elastic Band (CI-NEB) method is utilized to identify the transition state of the catalytic fixation mechanism.

Keyword: *CO2, SO2, and NO2 adsorption and utilization, MOFs, DFT, GCMC, CI-NEB*

Publications:

1. **Muthukumar Devaraj,** C.M.Nagaraja, Michael Badawi, and Renjith S. Pillai, "Computer modelling of trace SO2 and NO2 removal from flue gases by utilizing Zn(II) MOF catalysts", New Journal of Chemistry, 47, 2023, 18086-18095. (https://doi.org/10.1039/D3NJ01805A).
2. **Muthukumar Devaraj,** Athulya S. Palakkal, and Renjith S. Pillai, "Prediction of the capture and utilization of atmospheric acidic gases by azo-based square-pillared fluorinated MOFs," Physical Chemistry Chemical Physics, 25, 2023, 30458–30468. (https://doi.org/10.1039/D3CP02365F).
3. **Muthukumar Devaraj,** Sunaja Devi Kalathiparambil Rajendra Pai, Michael Badawi, and Renjith S. Pillai, "Molecular simulation prediction on SO2 gas adsorption in bipyridine ligand-based square-pillared mofs," ACS Applied Nano Materials, 7, 2024, 16630-16638. (https://doi.org/10.1021/acsanm.4c02680)