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Notice for the PhD Viva Voce Examination

Mr Sujith S, Registration Number: 2170242, 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, 06 May 2026 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 Solid Catalysts for Carbon Dioxide Activation and Conversion into Value Added Products**
Discipline	:	**Chemistry**
External Examiner - I	:	**Dr Benjaram Mahipal Reddy** Sr Professor Emeritus Department of Chemistry Birla Institute of Technology and Science, Pilani Hyderabad Campus, Jawahar Nagar Kapra Mandal, Medchal - 500078 Telangana
External Examiner - II	:	**Dr Ankur Bordoloi** Principal Scientist Catalytic Conversion and Process Division Council of Scientific and Industrial Research Indian Institute of Petroleum (CSIR-IIP) Dehradun, Uttarakhand - 248005
Supervisor	:	**Dr Sunaja Devi K R** Professor Department of Chemistry School of Sciences CHRIST (Deemed to be University) Bengaluru - 560029 Karnataka
Co-Supervisor	:	**Dr Ganapati V Shanbhag** Dean and Associate Professor (Former) Materials Science and Catalysis Division Poornaprajna Institute of Scientific Research Bengaluru - 562164 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.

Place: Bengaluru
Date: 17 April 2026

Registrar (Academics)

ABSTRACT

The growing need for sustainable chemical technologies has accelerated the exploration of carbon dioxide (CO_2) as a renewable C_1 feedstock. In this work, three distinct CO_2-related transformations, cycloaddition, carbonylation, and selective oxidation were investigated to design defect-engineered catalysts capable of efficient CO_2 activation and utilization. The selected reactions include: (i) cycloaddition of 1,2-propanediol (PD) to propylene carbonate (PC), (ii) carbonylation of monoethanolamine (MEA) to 2-oxazolidinone (2-Ox), and (iii) soft oxidation of furfural (FA) to furoic acid (FO). For the cycloaddition reaction, Cu-Mo mixed oxides were synthesized, with $Cu_3Mo_2O_9$ prepared at 500 °C showing a high density of oxygen vacancies and metastable Cu^+/Mo^{5+} species. These defect sites created cooperative Lewis acid–base pairs that facilitated strong CO_2 chemisorption, as supported by structural characterization and theoretical analyses (DFT, COHP, and ELF). The optimized catalyst delivered 99% PD conversion and 97% PC yield with excellent recyclability. In the MEA carbonylation reaction, Zn-NC catalysts derived from ZIF-8 were tuned via controlled pyrolysis. The Zn-NC-550 °C sample exhibited an optimal distribution of $Zn\text{-}N_4C$ and frustrated Lewis pair (FLP, $Zn\text{-}N_{4\text{-}x}C$) sites. Spectroscopic and temperature-programmed analyses confirmed the nature and density of these active centers. Computational studies indicated that COOH-containing intermediates preferentially adsorb at FLP sites, steering the reaction toward selective 2-Ox formation, whereas alternative binding modes led to side products. Site-blocking experiments further verified the critical role of FLPs. For furfural oxidation, CeO_2 nanocatalysts prepared via hydrothermal and MOF-derived routes were compared. The MOF-derived CeO_2-NF-MOF demonstrated superior activity due to enriched Ce^{3+} species and oxygen vacancies, resulting in enhanced reducibility and balanced surface acidity. Spectroscopic evidence confirmed favorable substrate adsorption, leading to 99.9% conversion and selectivity with sustained stability. This study establishes a unified strategy for defect engineering in heterogeneous catalysis, demonstrating how tailored electronic and structural features can drive efficient CO_2 activation across chemically diverse transformations.

Keywords: *CO_2 activation, CO_2 Utilization, Lewis Pair Sites, Biomass, 1,2-propanediol, Propylene carbonate, Furoic acid, Furfural, 2-oxazolidinone, Oxygen Vacancies, Nitrogen Vacancies, DFT, Defect sites, CDD, ELF, COHP.*

Publications:

1. **S. Sujith**, B. J. Vaishnavi, K. M. Rajashekhar Vaibhava, Kalathiparambil Rajendra Pai Sunajadevi, Ganapati V. Shanbhag "Utilizing Highly Reactive Lewis Pairs Generated by Oxygen Vacancies in the $Cu_3Mo_2O_9$ Solid Catalyst for Cycloaddition of CO_2 to 1,2-Propanediol", ACS Inorganic Chemistry, 2025, 64, 25, 12473–12491. https://pubs.acs.org/doi/10.1021/acs.inorgchem.5c00316
2. **S. Sujith**, H.K. Meghana, M. Harsha, B. J. Vaishnavi, Chaitra N. Mallannavar, Kalathiparambil Rajendra Pai Sunajadevi, Ganapati V. Shanbhag "Harnessing MOF Derived Frustrated Lewis Pair-CeO_2 Nano Catalyst for CO_2-Activated Soft Oxidation of Furfural to Furoic Acid", Chemistry-A European Chemistry, December, 2025. https://doi.org/10.1002/chem.202502616