

**CHRIST**(DEEMED TO BE UNIVERSITY)  
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## Notice for the PhD Viva Voce Examination

Ms Malavika S Kumar, Registration Number: 2270124, PhD Scholar at the Department of Chemistry, School of Sciences, CHRIST (Deemed to be University) will defend her PhD thesis at the public viva-voce examination on Monday, 30 March 2026 at 02.00 pm in Room No. 044, Ground Floor, R&D Block, CHRIST (Deemed to be University), Bengaluru - 560029, Karnataka, India.

<b>Title of the Thesis</b>	:	<b>Design and Synthesis of Fluorescent Chemosensors for the Selective Detection of Biorelevant Metal Ions and Reactive Species</b>
<b>Discipline</b>	:	<b>Chemistry</b>
<b>External Examiner - I</b>	:	<b>Dr Sib Sankar Mal</b> Associate Professor National Institute of Technology Srinivasnagar, Surathkal Mangaluru - 575025 Karnataka
<b>External Examiner - II</b>	:	<b>Dr Swapan Dey</b> Associate Professor Department of Chemistry and Chemical Biology Indian Institute of Technology (Indian School of Mines) Sardar Patel Nagar, Kalyanpur Dhanbad - 826007 Jharkhand
<b>Supervisor</b>	:	<b>Dr Avijit Kumar Das</b> Associate 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.

Place: Bengaluru  
Date: 17 March 2026

Registrar (Academics)

## ABSTRACT

This thesis details the design and application of a series of fluorescent chemosensors for critical analytes in security, environmental, and biomedical fields. The work begins with developing probes DPBO and ADM for sensitive phosgene detection via specific reaction mechanisms, validated in soil and household matrices. It progresses to multifunctional sensors: NCP, which integrates AIE and viscosity response to detect  $\text{OCl}^-$  and  $\text{Cu}^{2+}$ , while IMA detects  $\text{OCl}^-$  and  $\text{Zn}^{2+}/\text{Mn}^{2+}$  via separate signaling pathways. For environmental monitoring, the AMN dyad uses ESIPT modulation to sense picric acid (PA) and ammonia. The research culminates in the DHN probe, which combines AIE with a double proton-transfer (ESIDPT) mechanism for ultra-sensitive PA/ $\text{OCl}^-$  detection and is successfully engineered into a practical 3D-printed sensor. Overall, this work demonstrates a strategic evolution from molecular design to the creation of deployable sensing platforms.

**Keywords:** *Chemosensors; Fluorescence; Metal ion detection; Reactive species sensing; Environmental monitoring; Molecular docking/DFT*

### Publications:

1. **Kumar, Malavika S.,** Vishnu S, Malay Dolai, Anish Nag, Yatheesharadhya Bylappa, and Avijit Kumar Das. 2024. "Viscosity-Sensitive and AIE-Active Bimodal Fluorescent Probe for the Selective Detection of  $\text{OCl}^-$  and  $\text{Cu}^{2+}$ : A Dual Sensing Approach DFT and Biological Studies Using Green Gram Seeds." *Analytical Methods* 16 (5): 676–85.
2. **Kumar, Malavika S.,** Malay Dolai, and Avijit Kumar Das. 2024. "A Rapid and Selective 'on-off' Fluorescence Detection of Lethal Pulmonary Agent Phosgene Supplemented with Theoretical Approach: A Cost-Effective Sensing Tool for Household Bleach and Soil Analysis." *New Journal of Chemistry* 48 (20): 9103–9.
3. **Kumar, Malavika S.,** and Avijit Kumar Das. 2024. "'On-off' Fluorescence Detection of Exposed Phosgene via Pyrazine Ring Formation on a Triphenyl Amine Backbone Supplemented with a Theoretical Approach and Practical Environmental Applications." *New Journal of Chemistry* 48 (31): 13776–82.
4. **Kumar, Malavika S.,** Avijit Kumar Das, Yatheesharadhya Bylappa, and Anish Nag. 2025. "Selective Dual-Mode Detection of Reactive Oxygen Species and Metal Ions by Chemodosimetric Chelation Pathways: Fluorescence 'Turn-on' with  $\text{OCl}^-$  and  $\text{Zn}^{2+}/\text{Mn}^{2+}$ , Employing Theoretical, Practical, and Bioimaging Applications." *RSC Advances* 15 (9): 6708–17.
5. **Kumar, Malavika S.,** Sourav Pakrashy, Sounik Manna, Sujata Maiti Choudhury, Bhiguram Das, Abhishek Ghosh, Asiful H. Seikh, Malay Dolai, and Avijit Kumar Das. 2025. "Fluorogenic Selective Detection of  $\text{Zn}^{2+}$  Using a Pyrazole--Vanillin Conjugate: Insights from DFT, Molecular Docking, Bioimaging and Anticancer Applications." *Analytical Methods* 17 (9): 2125–33.
6. **Kumar, Malavika S.,** and Avijit Kumar Das. 2025. "A Dual-Fluorescence Approach for Turn-on Ammonia and Turn-off Explosive Picric Acid Detection ESIPT Inhibition: Experimental, Theoretical, and Biological Studies." *RSC Advances* 15 (39): 32894–32905.