

Notice for the PhD Viva Voce Examination

Ms Anitha Abraham, Registration Number: 2170202, PhD Scholar at the Department of Physics and Electronics, School of Sciences, CHRIST (Deemed to be University), Bangalore will defend her PhD thesis at the public viva-voce examination on Friday, 26 September 2025 at 2.00 pm in Room No. 044, Ground Floor, R & D Block, CHRIST (Deemed to be University), Bengaluru - 560029, Karnataka, India.

Title of the Thesis : Transition Metal-Based Nanocatalysts from MOF

and 2D Materials for Hydrogen Production from

Chemical Hydrides

Discipline : Physics

External Examiner - I : Dr Antonio Miotello

Senior Professor

Physics Department University of Trento

Via Sommarive

14, 38123 Povo (Trento)

Italy

External Examiner - II : Dr M Ariyanandhan

Professor

Centre for Nanoscience and Technology

Anna University Chennai - 600025 Tamil Nadu

Supervisor : Dr Rohan Pascal Fernandes

Associate Professor

Department of Physics and Electronics

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: 15 September 2025

Registrar (Academics)

ABSTRACT

World energy needs are increasing due to the rapid rise of industrialization, technology, and the increase in global population. The disparity between the supply of energy and the energy demand can't be contained and is growing out of control. With negative environmental issues and severe energy deficiency owing to the ongoing depletion of traditional fossil fuels, there is a need for new sources of energy that can substitute conventional existing energy resources. Hydrogen has been deemed one of the most suitable renewable energy carriers due to its advantages, including high energy density and clean emission. Chemical hydrides are a means of storing and releasing hydrogen at near-ambient temperatures and pressures. Among chemical hydrides, sodium borohydride (NaBH4) plays a special role due to the high H2 content, reasonable cost, and stability of their alkaline solutions. The hydrolysis of Sodium borohydride in the presence of suitable catalysts releases a significant volume of pure hydrogen gas. The byproducts can be recycled and are harmless to the environment. Seeking appropriate non-noble metal-based catalysts is a vital step needed to improve the sluggish kinetics of the hydrolysis process. The main aim of this work is to develop novel, low-cost transition metal-based nanocatalysts from Metal-organic frameworks (MOFs) and two-dimensional materials for hydrogen production from the hydrolysis of Sodium borohydride (NaBH4). In developing a catalytic system for hydrogen generation, we initially focused on Cobalt-based metal-organic frameworks, namely CoB, CoPB-MOF, and CoNiPB-MOF. It was synthesized through a simple hydrothermal method and tested its Hydrogen generation rate. The HGR produced by CoB-MOF, CoPB-MOF, and CoNiPB-MOF is found to be 1.8, 3.6, and 5.2 L/min/gm, respectively. The promising catalytic activity of MOFs could be attributed to their high surface area, the presence of cobalt active sites, and the synergic effects of P and B.

Advancing from the promising catalytic activity of MOFs and further enhancing the catalytic efficiency, nanostructured catalysts like nanocubes (3D), nanorods (1D), and nanosheets (2D) are explored. They demonstrated even higher HGR than that of Cobalt-based MOFs at lower activation energy due to its controlled morphology, and size effect at nanoscale which alter the electronic properties. Besides they also provide a higher surface area to volume ratio compared to the bulk materials.

Since these catalysts are in powder form and face problems in complete recovery and practical applications, finally, nickel foam, which has a three-dimensional porous structure, is used as catalyst support to solve these issues. A simple yet novel molten salt synthesis was employed to develop this new CoB/NF and CoPB/NF catalyst. The CoPB/NF could generate an HGR of ~14.2 L/min/gm at an activation energy (Ea) of 16.1 KJ/mol. This value is comparable with the HGR of noble metals like Ru NP/C (15.5 L/min/gm). The newly synthesized catalyst was utilized to regulate hydrogen production through an ON/OFF switching mechanism. This research opens up new possibilities for the development of phospho-boride-based materials for the hydrolysis of NaBH4 and the design of a hydrolysis reactor with improved performance for industrialization.

Keywords: Hydrolysis, NaBH4, Metal-organic framework, nanostructures, nano-catalysi, hydrogen generation

Publications:

- 1. **A Abraham**, R Silviya, R Patel, N Patel, R Fernandes "MOF derived cobalt-phospho-boride for rapid hydrogen generation via NaBH4 hydrolysis". Int. Journal of Hydrogen Energy, Vol.77, 2024, p. 1245-1253 oi.org/10.1016/j.ijhydene.2024.06.247
- A Abraham, S. Gupta, R Patel, N Patel, R Fernandes "Surface modified Cobalt Oxide Nanostructures for Hydrogen Generation from catalytic dissociation of NaBH4", FUEL, Vol. 395, 2025, p. 135198 doi.org/10.1016/j.fuel.2025.135198