

Notice for the PhD Viva Voce Examination

Ms Silviya R (Registration Number: 2071212), PhD Scholar at the School of Sciences, CHRIST (Deemed to be University), Bangalore will defend her PhD thesis at the public viva-voce examination on Friday, 16 May 2025 at 2.00 pm in Room No. 044, Ground Floor, Research and Development Block, CHRIST (Deemed to be University), Bengaluru - 560029.

Title of the Thesis : **Realizing Nanostructured Transition Metal Compound Electrocatalyst for H₂ Production by Seawater Electrolysis**

Discipline : **Physics**

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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: 08 May 2025



Registrar

ABSTRACT

Using intermittent power from renewable sources (solar and wind) for electrolysis water to produce hydrogen and oxygen offers a sustainable and eco-friendly way to store and transmit energy for on-demand applications. The primary emphasis is creating effective and affordable electrolyzers using highly pure water feed. The global scarcity of freshwater resources has recently driven the need to explore abundant seawater as an alternative feedstock for hydrogen production by water-splitting. This route comes with new challenges for the electrocatalyst, which has to withstand harsh saline water conditions with selectivity towards oxygen evolution over other competing reactions. In this work, the focus is to develop a low-cost transition metal electrocatalyst via facile synthesized techniques. Co-B, Ni-B, and Fe-B, the mono-metallic borides, are tested in alkaline simulated seawater. Among them, the Co-B electrocatalyst shows low overpotential values for OER (305 mV) and HER (182 mV), respectively. Several approaches revealed that the in-situ surface alteration (OER) and enrichment of the metal site with excess electrons (HER) are responsible for this improved activity. To further enhance the characteristics of these nanoparticles, a sequence of amorphous transition-metal phospho-borides, are synthesized using a chemical reduction technique and evaluated for their ability to facilitate alkaline seawater electrolysis.

The addition of P in Co-B has increased the optimal electron density on the metal sites which has been proven both experimentally and theoretically. Likewise, the effect of dopants is examined by supplementing the optimized electrocatalyst Co-P-B with another earth-based abundant transition metal ($M = \text{Cu, Ni, Fe, W, Mo, V, \& Mn}$). The bimetals that have been alloyed with P and B contribute to regulating the electron density at active metal sites. In alkaline simulated seawater, CoMoPB and CoFePB catalysts outperform Co-P-B with the lowest overpotential (η_{10}) of 56 mV (HER) and 264 mV (OER), respectively. Additionally, the CoWPB electrocatalyst exhibits bifunctional activity along with an excellent corrosion-resistant property in seawater conditions. Finally, nitrogen-doped carbon (NC) incorporated CoMoPB and CoFePB catalysts were tested in seawater. The appropriate NC doping helps in the increase the surface area and conductivity. The synthesized CoMoPB/NC demonstrated HER activity with the lowest overpotential (η_{10}) value of 43 mV in comparison to the standard electrocatalyst (Pt/C, $\eta_{10} = 56$ mV), exhibiting better durability over 50 hours at 100 mA/cm². For OER, a minimal value of ~ 248 mV at 10 mA/cm² is observed in the CoFePB/NC electrocatalyst. This work offers a cost-effective approach for producing hydrogen via seawater electrolysis and would open up new avenues to the design and development of phospho-boride-based material towards electrocatalyst application with enhanced performance for commercialization.

Keywords: Seawater electrolysis, Electrocatalyst, Bifunctional, Hydrogen evolution reaction, Oxygen evolution reaction, Green hydrogen

Publications:

1. **R. Silviya**, Yashashree Vernekar, Aniruddha Bhide, Suraj Gupta, Nainesh Patel, and Rohan Fernandes, Non-Noble Bifunctional Amorphous Metal Boride Electrocatalysts for Selective Seawater Electrolysis, *ChemcatChem*, 2023, Wiley VCH, 15 (17), e20230063, <https://doi.org/10.1002/cctc.202300635>.
2. **R. Silviya**, Aniruddha Bhide, Suraj Gupta, Rinkoo Bhabal, Kishan H. Mali, Brajesh Rajesh Bhagat, Matjaž Spreitzer, Alpa Dashora, Nainesh Patel, and Rohan Fernandes, Bifunctional Amorphous Transition-Metal Phospho-Boride Electrocatalysts for Selective Alkaline Seawater Splitting at a Current Density of 2A cm⁻², *Small methods*, 2024, Wiley VCH, 2366-9608, 2301395 <https://doi.org/10.1002/smt.202301395>