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Notice for the PhD Viva Voce Examination

Mr Aniruddha Santosh Bhide (Registration Number: 2170021), PhD Scholar at the School of Sciences, CHRIST (Deemed to be University), Bangalore Central Campus will defend his PhD thesis at the public viva-voce examination on Tuesday, 15 April 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	:	**Developing Non-Noble Electrocatalyst for H_2 Production by Effective Water and Urea Oxidation**
Discipline	:	**Physics**
External Examiner (Outside Karnataka)	:	**Dr Pravin Sadashiv More** Professor Department of Physics Application laboratory The Institute of Forensic Science 15, Madam Cama Road Mumbai - 400032, Maharashtra
External Examiner (Within Karnataka)	:	**Dr Aninda Jiban Bhattacharyya** Professor Interdisciplinary Centre for Energy Research Solid State and Structural Chemistry Unit Indian Institute of Science Bengaluru - 560012, Karnataka
Supervisor	:	**Dr Nainesh Kantilal Patel** 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.

Registrar

Place: Bengaluru
Date: 07 April 2025

ABSTRACT

The current energy sector is dominated by fossil fuel-based energy carriers, which contribute to severe environmental problems. As an alternative, green hydrogen has emerged as a promising energy carrier for storing excess energy. However, the large-scale adoption of hydrogen as a fuel is hampered by the necessity of high cost of noble-metal-based electrocatalysts. This thesis aims to address this limitation by developing cost-effective, transition metal (TM)-based nanomaterials with catalytic performance and stability suitable for scalable water-splitting applications. Initially, an amorphous CoWPB was explored as a bifunctional electrocatalyst. For both hydrogen evolution reaction (HER) and oxygen evolution reaction (OER), optimized compositions of CoWPB achieved overpotentials of 72 mV and 262 mV respectively, while a cell potential of 1.59 V was required in a two-electrode setup at 10 mA/cm2 using 1 M KOH. Robustness tests, including a 70-hrs stability and 10,000-cycle recyclability, demonstrated the catalyst's durability. Computational and electrochemical studies indicated that the inclusion of W enhanced surface area and conductivity, while B-modulated P and Co sites served as active sites for HER and OER, respectively. A subsequent study focused on improving the sluggish OER where the B and P-incorporated cobalt-oxide nanowires (B/P-CoOx NW) were investigated. The B/P-CoOx NW showed an impressive overpotential of 230 mV at 10 mA/cm2, comparable to top-performing electrocatalysts in the literature. The presence of oxygen vacancies (Ov) led to a phase transition from Co3O4 to CoO, enhancing each step of the OER mechanism, as revealed by detailed in-situ electrochemical kinetic analysis. The B/P-CoOx NW exhibited excellent robustness with stability lasting 80 hours and cyclability of 10,000 cycles.

Following the nanowires, two-dimensional B/P-CoOx nanosheets (NS) were synthesized and evaluated for their OER performance. The B/P-CoOx NS exhibited outstanding activity, achieving an even lower overpotential of just 220 mV at 10 mA/cm2. In addition to Ov, the nanosheets contained multidimensional defects that contributed to enhanced conductivity, improved catalytic activity, and the structural conversion from Co3O4 to CoO. Minimal activity loss was observed in a 100-hrs chronoamperometric test. In a zero-gap single-cell alkaline electrolyzer setup operating in 6 M KOH at 60°C, the system reached a current density of 500 mA/cm2 at only 1.76 V, demonstrating strong industrial feasibility. Splitting natural urine through a urea oxidation reaction (UOR) instead of OER requires less energy offering an economical alternative to pure water splitting. Thus, in the final work, B/P-CoOx nanostructures deposited on nickel foam (NF) were tested for the UOR. The B/P-CoOx NW/NF required a UOR potential of only 1.33 V to achieve 50 mA/cm2 in synthetic urine, demonstrating excellent performance. When natural cow urine was used as the electrolyte, the catalytic activity only slightly degraded, requiring 1.35 V at 50 mA/cm2. Kinetic studies revealed that abundant active site formation, improved adsorption kinetics, and rapid CO2 desorption contributed to the superior UOR activity. Additionally, the catalyst exhibited stability for 100 hours and retained its performance through 10,000 cycles. In conclusion, this thesis provides valuable insights into the design, synthesis, and evaluation of TM-based electrocatalysts for both water and urea splitting.

Keywords: *HER, OER, Urea splitting, Phospho-borides, Oxygen vacancy, Crystalline defects, Kinetic study*

Publications:

1. **Bhide, A.**; Gupta, S.; Bhabal, R.; Mali, K. H.; Bhagat, B. R.; Dashora, A.; Patel, M.; Fernandes, R.; Patel, N. Unveiling the Synergistic Effect of Amorphous CoW-Phospho-Borides for Overall Alkaline Water Electrolysis. Int. J. Hydrogen Energy 2024, 63 (March), 645–656. https://doi.org/10.1016/j.ijhydene.2024.03.090
2. **Bhide, A.**; Gupta, S.; Bhabal, R.; Patel, M.; Bahri, M.; Fernandes, R.; Patel, N. Unveiling the Kinetics of Oxygen Evolution Reaction in Defect-Engineered B/P-Incorporated Cobalt-Oxide Electrocatalysts. Mater. Today Energy 2024, 44, 101638. https://doi.org/10.1016/j.mtener.2024.101638
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7. Silviya, R.; **Bhide, A.**: Gupta, S.: Bhabal, R.: Mali, K. H.: Bhagat, B. R.: Spreitzer, M.: Dashora, A.: Patel, N.: Fernandes, R. Bifunctional Amorphous Transition-Metal Phospho-Boride Electrocatalysts for Selective Alkaline Seawater Splitting at a Current Density of 2 A cm-2. Small Methods 2024, 2301395, 1-14. https://doi.org/10.1002/smtd.202301395
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9. Bhabal, R.; **Bhide, A.**; Gupta, S.; Fernandes, R.; Patel, N. Maximizing Bifunctionality for Overall Water Splitting by Integrating H2 Spillover and Oxygen Vacancies in CoPBO/Co3O4 Composite Catalyst. *Accepted in Small Science*
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