

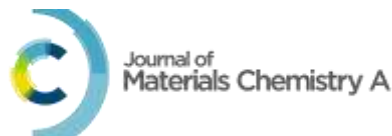
**Chem4Energy Annual Conference**  
**Materials and Processes for a Sustainable Energy Future**  
**Monday 7 – Friday 11 April 2025**



*Conference Programme (may be subject to amendment)*

**Monday 7 April 2025**

13:00 – 13:30	<i>Registration</i>	
13:30 – 13:40	<b>Welcome and Opening</b>	Professor Nora de Leeuw University of Leeds, UK; Utrecht University, The Netherlands
13:40 – 13:50	<i>Chair's comments</i>	<i>Professor Veikko Uahengo, University of Namibia, Namibia</i>
14:00 – 14:45	<b>Introductory Lecture</b>	<b>Dr Simeon Hamukoshi</b> <b>National Commission on Research, Science and Technology,</b> <b>Namibia</b>
14:45 – 15:15	<i>Refreshment Break</i>	
15:15 – 16:00	<b>Keynote</b> Extraction of critical minerals from copper-nickel concentrate: The role of coordination chemistry in the hydrometallurgical process	<b>Professor James Darkwa, University of Johannesburg, South Africa</b>
16:00 – 16:25	Photocatalytic Hydrogen Production via Cobalt Phthalocyanine Incorporated with Metal-Organic Framework	Dr Sheriff Balogun, University of Limpopo, South Africa
16:25 – 16:50	Computational and experimental studies of single atom alloy catalysts for NH <sub>3</sub> synthesis	Professor Geoffrey Njovu, University of Oxford, UK
16:50 – 17:05	Photocatalytic H <sub>2</sub> evolution by hydrothermally synthesized NaBH <sub>4</sub> - spiked ZnS nanostructures	Theopolina Amakali, University of Namibia
17:05 – 17:15	Poster 2-minute flash presentations	Professor Marile Landman, University of Pretoria, South Africa Rotondwa Mphedu, University of the Witwatersrand, South Africa Professor Liezel van der Merwe, University of Pretoria Dr Marrigje Marianne Conradie, University of Free State, South Africa
17:15 – 18:30	<b>Poster Session</b>	
18:30	<i>Close of session</i>	



# Extraction of Critical Minerals from Copper-Nickel concentrate: The role of coordination chemistry in the hydrometallurgical process

James Darkwa\*

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## Introduction

There are several reports about sub-Saharan Africa being at the centre of global critical minerals production. One such report is by Chen *et al.* entitled “Harnessing Sub-Saharan Africa’s Critical Mineral Wealth,”<sup>1</sup> but none of these reports is on the beneficiation of these minerals to the grade and purity of compounds for which the world seeks these critical minerals from Africa. Is it because the chemistry needed to beneficiate these critical minerals to the desired materials too difficult for Africa? This presentation will provide answers to this question.

## Materials and Methods

Acid leaching was used to extract critical metal salts from copper-nickel concentrates. Treatment of the leachate with different classical solvent extraction reagents were performed to extract copper, nickel, and cobalt salts in >90% selectivity; and precipitated in highly pure forms.

## Results and Discussion

Results from this study shows how using low acid concentration and the appropriate extraction solvent demonstrates that the simplicity and effectiveness of coordination chemistry in hydrometallurgy. So, one wonders why, with these tools that are provided by coordination chemistry, Africa is still seen as a place where ores are taken from to other places where extraction is performed.

## References

1. W. Chen, A. Laws and N. Valckx, *IMF News*, April 29, 2024.
2. B. Chandler, *Mo Ibrahim Foundation Report*, October 2020.

# Photocatalytic Hydrogen Production via Cobalt Phthalocyanine Incorporated with Metal-Organic Framework

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## Introduction

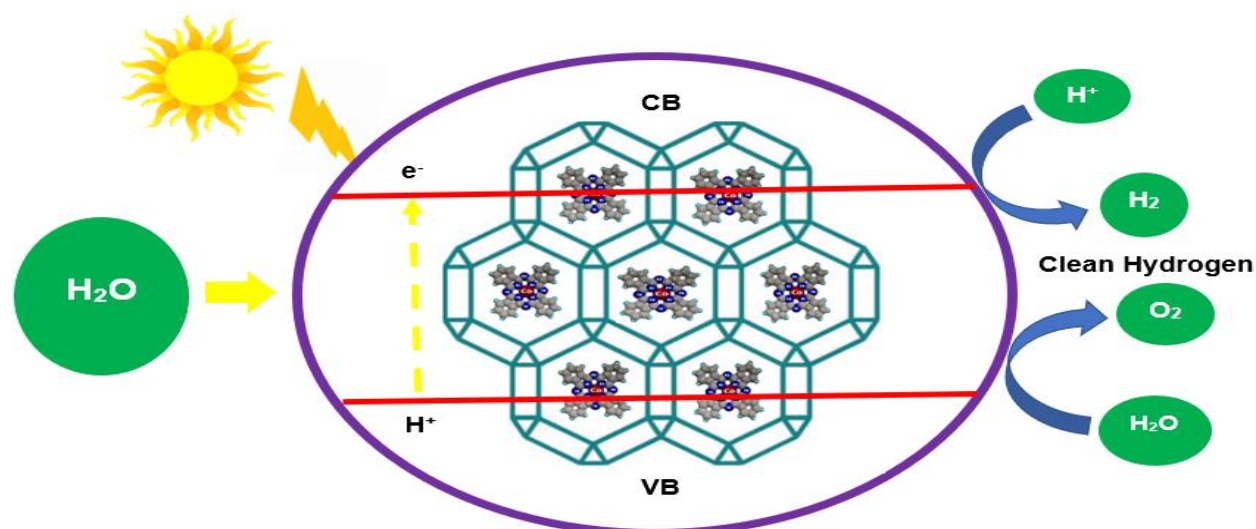
The quest for efficient and sustainable hydrogen production as an alternative energy source to lessen the impact of fossil fuels has led to extensive research into novel photocatalytic materials.<sup>1-3</sup> In this study, we investigate the photocatalytic hydrogen production performance of cobalt phthalocyanine (CoPc) incorporated with a metal-organic framework (MOF).

## Materials and Methods

The synthesized CoPc-MOF composite will be characterized using various analytical techniques such as XRD, SEM, UV spectroscopy, TGA, and FTIR. The electrochemical performance of the CoPc-MOF catalyst will be investigated using CV, LSV, CA, and EIS to reveal the remarkable photocatalytic properties of the composite for hydrogen evolution reaction (HER).

## Results and Discussion

The synergistic effects of these materials (CoPc and MOF) coupled with the MOF's flexible structure, ultra-large surface area, and tunable structural components, as well as the unique light absorption performance of the CoPc near infrared region promise to offer an excellent photocatalytic performance with increased active sites, improved charge transfer kinetics, and enhanced stability. This novel catalyst promises to be an efficient photocatalyst for high yield of hydrogen, hence offering insights into the design of advanced materials for renewable energy applications.



## References

1. S.A. Balogun, et al., *Advanced Energy and Sustainability Research*, (2024), 2400169.
2. M.D. Makhafola, et al., *Energies*, 17(7), (2024).1646.
3. S. Xu, et al., *Journal of Rare Earths*, 42(5), (2024), 838-850.

# Computational and experimental studies of single atom alloy catalysts for NH<sub>3</sub> production

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## Introduction

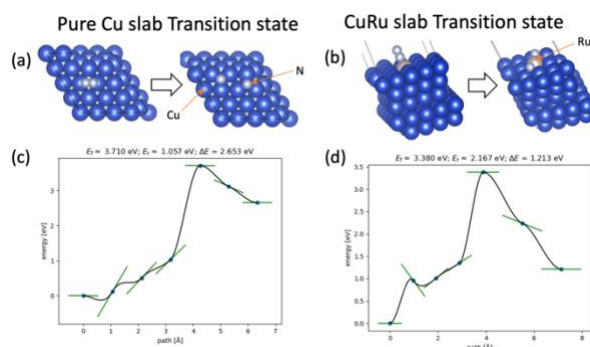
Single atom alloy (SAA) catalysts are a promising family of heterogeneous catalysts. They are composed of a PGM such as Pd, Pt, Ru & Rh atomically dispersed on the surface of a coinage metal such as Ag, Au and Cu (see **Figure 1**).<sup>1</sup> The host-dopant surface creates a synergistic geometric and chemical environment that leads to improved selectivity, activity and resistance to poisoning.<sup>1</sup> Herein, such catalysts are studied in the context of NH<sub>3</sub> production. With emerging uses of NH<sub>3</sub> as an energy vector and low carbon fuel, its demand is expected to more than triple from the current ~200 Mtpa production volume.<sup>2,3</sup> SAA catalysts can play an important role in NH<sub>3</sub> synthesis at milder conditions, unlocking a decentralised and energy efficient Haber Process.

## Materials and Methods

To model the performance of SAA catalysts in NH<sub>3</sub> synthesis, Density Functional Theory (DFT) and Machine Learning were employed to study the N<sub>2</sub> dissociation behaviour of a CuRu SAA catalyst surface (Cu host, Ru dopant) relative to a pure Cu surface. **Computational setup:** A 4x4x1 5-layer slab of Cu (111) was used in these calculations as Cu is a face centred cubic crystal system. The DFT calculations were performed using the Vienna Ab initio Simulation Package (VASP version 6) using the PBE functional and a cutoff energy of 400 eV.

## Results and Discussion

Firstly, the N<sub>2</sub> binding mode changes from side-on on the pure Cu surface to end-on on the CuRu surface (**Figure 1 a & b**). Secondly, the SAA catalyst (CuRu) significantly lowers the N<sub>2</sub> dissociation energy relative to pure Cu from 2.6 eV to 1.2 eV, a reduction equivalent to ~138 kJmol<sup>-1</sup> (**Figure 1 c & d**). These observations confirm that the introduction of one Ru atom materially changes the Cu structure and its behaviour towards N<sub>2</sub> dissociation, making N<sub>2</sub> scission more energetically favourable. Going forward, more dopant-host combinations will be modelled, with the most promising combinations synthesised and experimentally tested for NH<sub>3</sub> synthesis.



**Figure 1(left):** N<sub>2</sub> dissociation (the rate determining step in NH<sub>3</sub> synthesis) energetics on a CuRu SAA surface relative to a pure Cu surface. The former is more energetically favourable by about **1.4 eV (~138 kJmol<sup>-1</sup>)**, indicating that SAA structures can provide a potential route towards rational synthesis of high-performance NH<sub>3</sub> synthesis catalysts that are compatible with the intermittent supply of electrical energy such as wind and solar.

## References

1. Hannagan, R.T., et al., *Chemical Reviews*, 120(12), 2020, p.120144-12088.
2. Giddey, S., et al., *ACS Sustainable Chemistry & Engineering* 5(11), p.10231-10239.
3. International Energy Agency, *Ammonia Technology Road Map*, 2021.

# Photocatalytic H<sub>2</sub> evolution by hydrothermally synthesized NaBH<sub>4</sub>-spiked ZnS nanostructures

Theopolina Amakali<sup>1\*</sup>, Aleksandar Živković<sup>2,3,4</sup>, Michael E. A. Warwick<sup>5</sup>, Daniel R. Jones<sup>5</sup>, Charles W. Dunnill<sup>5</sup>, Likius S. Daniel<sup>1\*\*</sup>, Veikko Uahengo<sup>1</sup>, Claire E. Mitchell<sup>2</sup>, Nelson Y. Dzade<sup>2</sup>, Nora H. de Leeuw<sup>2,3,6</sup>

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## Introduction

The H<sub>2</sub> evolution via water splitting using a photocatalyst is an effective and ecofriendly technique to produce green hydrogen.<sup>1</sup> Semiconductor-mediated photocatalysis owes its popularity to a number of advantages including low cost, simplicity, and ease of preparation.<sup>2</sup> Zinc sulphide (ZnS) has particularly attracted much attention, owing to its suitable and tunable band gap position.

## Materials and Methods

In this study, samples of ZnS were prepared and doped via a hydrothermal route using different amounts of NaBH<sub>4</sub> (0 mol, 0.003 mol, 0.005 mol, 0.01 mol, 0.02 mol). The photocatalytic activity of the prepared ZnS samples was evaluated for hydrogen generation via the water splitting reaction under visible light irradiation.

## Results and Discussion

The declining photocatalytic activity of the prepared ZnS samples was observed with the increasing amount of NaBH<sub>4</sub> added. The amount of H<sub>2</sub> generated ranged from 1.3×10<sup>5</sup> μmol/g to 2.6 ×10<sup>5</sup> μmol /g under 9 h of visible irradiation for the samples treated with the 0.02 mol NaBH<sub>4</sub> and 0 mol NaBH<sub>4</sub>, respectively. The addition of NaBH<sub>4</sub> to ZnS samples prepared in this study did not improve the generation of H<sub>2</sub> as reported by previous authors and this could be attributed to different sample morphologies that were observed under SEM.<sup>4</sup> The rate of production obtained is however still comparable to what has been reported in literatur.<sup>5</sup> The high rate of H<sub>2</sub> production obtained for untreated ZnS samples suggests that with further optimization and testing, ZnS can be a suitable and effective photocatalyst for H<sub>2</sub> evolution via water splitting.

## References

1. Z. Tai et al. *J. Colloid. Sci.* 628, (2022), 252-260
2. K. P. Gopinath, K. P. *J. Environ. Manage.* 270, (2020), 110906.
3. J. Xiong et al. *Chem. Commun.* 57, (2021), 8186-8189.
4. G. Wang et al. *Sci. Rep.* 5, (2015) 8544
5. S. Shahid et al. *Int. J. Hydrog. Energy.* 62, (2024), 1113-1138