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

Conference Programme (may be subject to amendment)

Thursday 10 April 2025

08:50 – 09:00	*Chair's comments*	*Professor Scott Woodley, University College London, UK*
09:00 – 09:45	**Keynote** Modelling defects in oxides and nitrides	**Professor Richard Catlow, University College London, UK**
09:45 – 10:10	First principles study of hydrogen adsorption on Fe_2CrSi (110) surface	Dr David Tshwane, Council for Scientific & Industrial Research, South Africa
10:10 – 10:25	Chicken eggshells as heterogeneous catalyst for biodiesel production from E.spicatum seeds oil	Hilaria Hakwenye, University of Namibia
10:25 – 10:40	DFT study of the mechanism of water splitting on $CuWO_4$ surface	Xuan Chu, University of Leeds, UK
10:40 – 11:10	*Refreshment break*	
11:10 – 11:35	Percolation Threshold for the Photocatalytic Degradation of MB using unprecedentedly high concentrations of metallic silver nanoparticles in a ZnO thin film	Professor Likius Daniel, University of Namibia
11:35 – 12:00	Novel amino acid-based surfactants with intrinsic luminescence for UV down-conversion and enhanced solar energy efficiency	Dr Etienne Wiese, North-West University, South Africa
12:00 – 12:15	Optimization of biomass-derived activated charcoal supporting TiO_2 nanoparticles as a potential photocatalyst	Justine Auene, University of Namibia
12:15 – 12:30	Activated carbon from waste paper for the removal of contaminants from wastewater	Viola Willemse, University of Namibia
12:30 – 13:40	*Lunch*	
13:40 – 13:45	*Chair's comments*	*Dr Marietjie Ungerer*
13:45 – 14:10	DFT Modelling of Carbon Supported Platinum-Based Electrocatalysts	Professor Cornie van Sittert, North-West University, South Africa
14:10 – 14:25	Metal-organic framework modified carbon nanotubes for hydrogen production from formic acid	Dina Thole, University of Limpopo, South Africa
14:25 – 14:40	Removal of Contaminants from Wastewater with Activated Carbon from Acacia Erioloba Seed-Pods	Elia Haukongo, University of Namibia

Thursday 10 April 2025 continued

14:40 – 14:55	GH2-based ammonia-derived fertilizers, their application in desert soil fertility at Daures Village	Matilde Johannes, University of Namibia
14:55 – 15:20	Modelling the tautomerisation of model lignin molecules over zeolite MFI nanosheets	Professor Nora de Leeuw, University of Leeds, UK
15:20 – 15:50	*Refreshment Break*	
15:50 – 16:30	Discussion on Future Activities	All
16:30 – 16:45	Closing remarks	Professor Cornie van Sittert, North-West University, South Africa Professor Nora de Leeuw, University of Leeds, UK
16:45	*Close of Conference*	
18:30	*Conference Dinner*	*Hotel Restaurant*

New Insights into Defect and Electronic Properties of Oxides and Nitrides

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Modelling tools are well established in predicting defect and electronic properties of solid state ionic materials. Here we will highlight recent developments employing both Periodic Boundary Conditions Quantum Mechanical and Hybrid, Quantum Mechanical/ Molecular Mechanical (QM/MM) Methods(1), which are applied to widely studied oxide and nitride material, including CeO2, ZnO, AlN and GaN. Our approach allows is to develop models of defect and electronic structures which are consistent with and rationalise experimental data. We gain new insights into the role of surface structure in influencing defect and electronic properties), which we illustrate for the case of ceria(2. We predict charge carrier concentrations as a function of temperature and composition and are able to probe hole/electron - dopant interactions, where we discuss the factors controlling p-type conductivity in GaN(3).

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First principle study hydrogen adsorption on Fe_2CrSi (110) surface

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Introduction

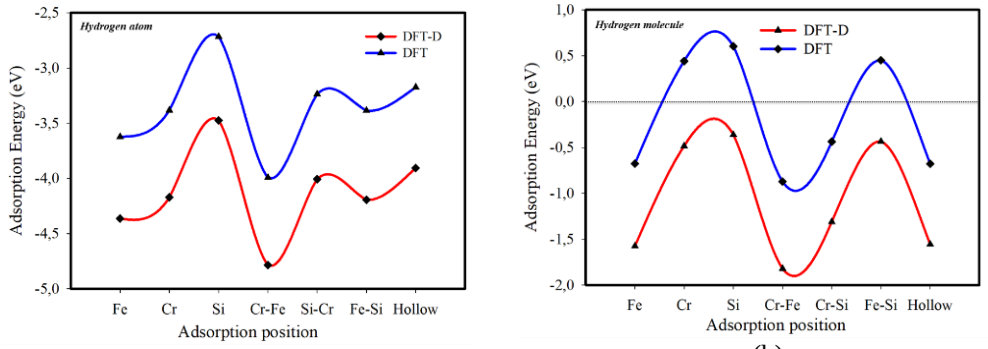
Ternary metallic alloys have received much attention in research and industry because they produce Intermetallic compounds with high strength and low density.[1] However, hydrogen embrittlement (HE) remains an obstacle with usage constraints, affecting materials' tensile strength, ductility, fracture strength, and toughness.[2, 3] This study analyses hydrogen adsorption on Fe_2CrSi surface.

Materials and Methods

The density functional theory calculations were performed using the CASTEP code employing plane-wave pseudopotential approach.[4] A comprehensive structure optimization and energy minimization computation were carried out using cutoff energy and Monkhorst-Pack k-points of 500 eV and 4x4x1, respectively.[5]

Results and Discussion

Figure 1 presents the hydrogen adsorption strength on the Fe_2SiCr surface at different adsorption position, namely, top of different atoms, bridge between two atoms and hollow sites. It was found that H atoms' adsorption energy is thermodynamically stable, with $E_{ads} < 0$ across all surface sites. For Fe_2SiCr alloy, the H adsorption energy strength at the top site was observed to follow the order of $E_{ads}^{Fe} > E_{ads}^{Cr} > E_{ads}^{Si}$.



(a) (b)

Figure 1: Depicts adsorption energies of (a) H atom and (b) molecule at different adsorption sites on Fe_2SiCr (110) surface.

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Chicken eggshells as heterogeneous catalyst for biodiesel production from *E.spicatum* seeds oil

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Introduction

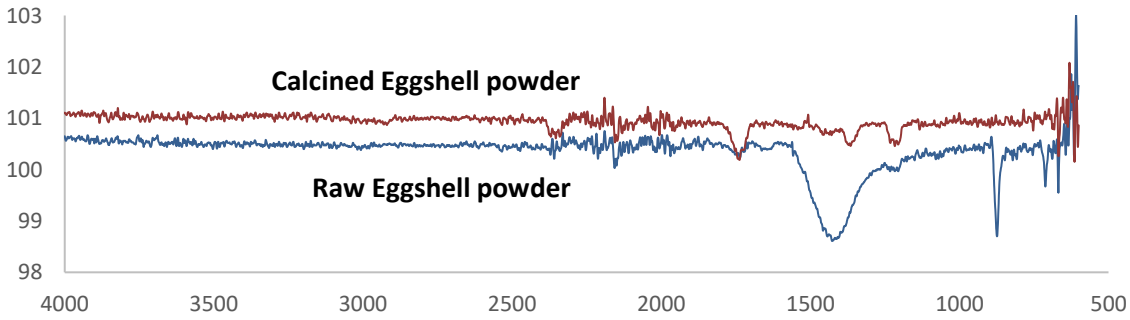
Heterogeneous catalysts are efficient, cost effective, reusable, facilitate facile recovery, and can be used at high temperatures[1]. In recent years, calcium oxide (CaO) has emerged as an efficient heterogeneous catalyst for biodiesel production[2]. However, the widespread use of commercial CaO may deplete its non-renewable resources[3]. Therefore, this study aimed to characterise CaO from waste eggshells for *Entandrophragma spicatum* seed oil transesterification.

Materials and Methods

Calcium carbonate was converted into CaO through calcination at high temperatures[4]. Different techniques, namely hydration-dehydration, decomposition, and sol-gel methods[5], were employed to prepare CaO catalysts with varying surface areas and active sites. The synthesised catalysts were characterised by Fourier Transform Infrared spectra (FTIR), the Hammett indicator method, and the yield and quality of biodiesel.

Results and Discussion

Raw eggshell FTIR spectra showed peaks representing the carboxylate ($CaCO_3$) group at 1420cm^{-1}, 873cm^{-1} and 713cm^{-1}, respectively which decreased or disappeared after calcination. Preliminary results from this study showed that the prepared catalyst can be used as a heterogeneous catalyst (CaO) for the sustainable production of biodiesel from E. spicatum seeds oil.



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Water adsorption at the (010) surfaces of $CuWO_4$

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Introduction

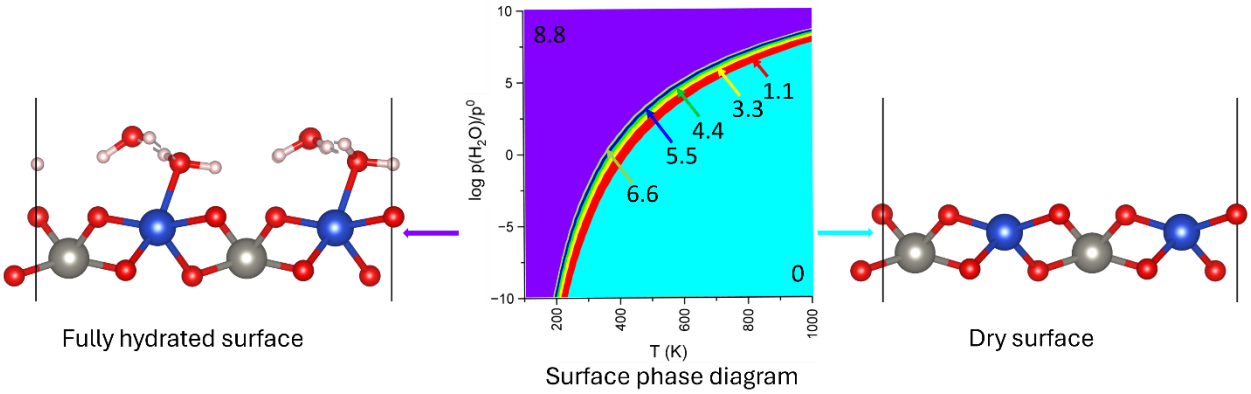
Copper tungstate ($CuWO_4$) has attracted significant attention over the past two decades. However, the adsorption of water onto $CuWO_4$, which plays a critical role in the photocatalytic water splitting process, has not been investigated in detail. In this study, we have employed density functional theory (DFT) calculations to investigate water adsorption onto the $CuWO_4$ pristine (010) surfaces.

Materials and Methods

In this work, we performed DFT calculations using the Vienna ab initio simulation package (VASP)[1]. The dipole method proposed by Tasker[2] was applied to construct the pristine low-Miller index surfaces. We employed the METADISE package[3] to construct the low-Miller index surfaces from the bulk phase of $CuWO_4$.

Results and Discussion

The single water adsorption mode with H_2O situated over Cu in μ_3-η^3 configuration has the largest adsorption energy of -0.89 eV. The surface can adsorb up to eight H_2O molecules can per surface cell. Four H_2O molecules bonded with Cu in the surface, whereas the other four interacted with neighbouring H_2O molecules via hydrogen-bonds, forming an ice-like monolayer over the surface. The results of phase diagram suggest that the (010) surfaces prefer to remain dry at low partial pressures of H_2O but can become fully hydrated at high partial pressures of H_2O at low temperatures.



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Percolation Threshold for the Photocatalytic Degradation of MB using Unprecedentedly High Concentrations of Metallic Silver Nanoparticles in a ZnO thin film.

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Introduction

Like other metal oxide photocatalysts, zinc oxide (ZnO) can mineralize organic dyes into water (H_2O), carbon dioxide (CO_2), and mineral acids, while avoiding the production of secondary pollutants[1]. In contrast to most metal oxide semiconductors, it has been observed that the enhancement of photo responsiveness of ZnO into the visible range using the chemical method of doping noble metals is challenging[2]. The investigation and analysis of degradation circumstances that impact the degradation of ZnO in relation to various azo bond dyes are deemed significant. This study is investigating how the Ag/ZnO ratio can be manipulated to enhance the photo responsiveness of ZnO, extending its range to the visible light region and beyond. The photocatalytic properties of the fabricated thin films were investigated to determine their impact on the rate of MB degradation.

Materials and Methods

The Ag-NP/ZnO composite (COMP-Ag_n; n = 20, 40, 50, 60, 70, 75 and 80 Ag mol%) thin films were fabricated by heat treating the spin-coated precursor films, while applying the composite solution with various concentrations adjusted in the range 10–80 mol% as reported by Daniel and his team[3]. The XRD, SEM, optical properties, photocatalytic properties of the fabricated thin films were measured.

Results and Discussion

The pure ZnO and seven Ag-NP/ZnO composite thin films were successfully fabricated on silica glass. The optical properties of the composite electrodes were investigated, and the results indicate that the incorporation of Ag NPs into the ZnO matrix did not result in any alteration of the band gap. The absorption bands detected within the wide wavelength range of 380 nm to 700 nm are ascribed to the surface plasmon resonance (SPR) absorption of electrons that are trapped within silver nanoparticles. The X-ray diffraction (XRD) spectra of ZnO and Ag-NP/ZnO composite thin were found to align with those of the standard ZnO (JCPDS 36-1451), indicating that the thin films possess the characteristic hexagonal wurtzite structure and metallic silver are impreganated into the ZnO matrix. The effectiveness of pure ZnO and Ag-NPs/ZnO thin films in the photodegradation of methylene orange (MO) and, tartrazine 85 (T85), rhodamine B (RhB), and DB38 demonstrated a gradual reduction of respective absorption bands over a 6-hour period, highlighting the significance of the photocatalyst in the photocatalytic degradation of dyes and determine the percolation threshold to be at 0.55 molar ratio of Ag-NP to ZnO.

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Novel Amino Acid-Based Surfactants with Intrinsic Luminescence for UV Down-Conversion and Enhanced Solar Energy Efficiency

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Introduction

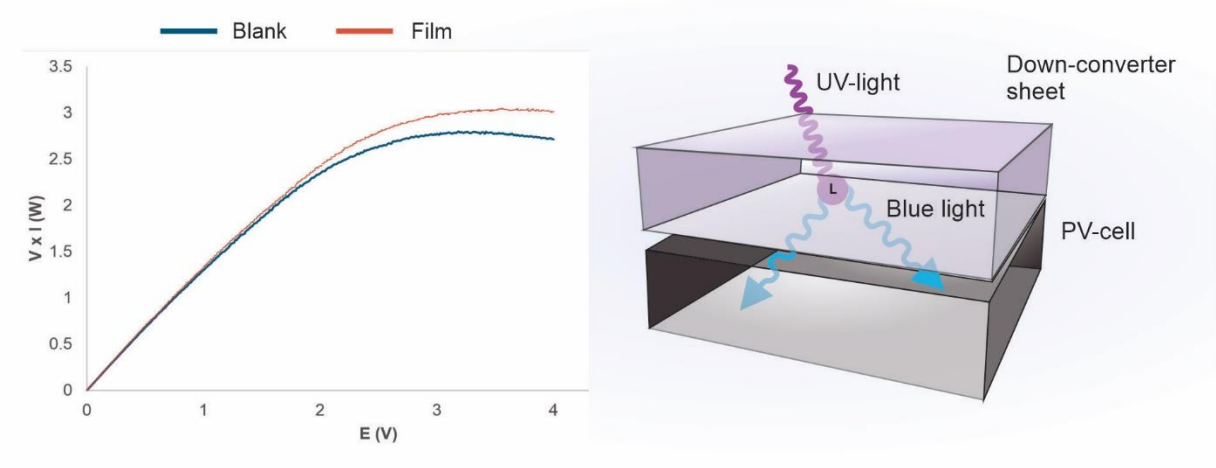
Advancements in the efficiency and lifespan of photovoltaic (PV) cells are essential to progress in solar energy technology. This study presents the synthesis and characterisation of novel Guerbet-type, amino acid-based surfactants, which are incorporated into a polymer matrix for use as ultraviolet (UV) downconverters. Such UV downconverter films can be applied either as aftermarket solar panel coating products or directly during PV cell manufacturing to improve solar conversion efficiency and extend the operational life of PV cells.

Materials and Methods

Amino acid-based surfactants were embedded within a PMMA matrix, with their optical properties characterised using UV-vis and fluorescence spectroscopy to confirm both intrinsic luminescence and UV down-conversion potential (Hsieh, Cheng et al. 2022, Wiese, Otto et al. 2024). To assess their effectiveness on PV cells, thin surfactant-polymer sheets were applied to PV modules, and their impact on solar conversion efficiency was evaluated using a solar simulator.

Results and Discussion

Optimal surfactant concentrations were identified to achieve full UV radiation filtering. Notably, aminobenzoic acid-based surfactants displayed significant structural influence, with the ortho isomer showing significantly higher UV down-conversion efficiency than the para isomer. The surfactants effectively down-converted UVA and UVC radiation to visible light, while a cosurfactant was required to down-convert UVB light. These results highlight the critical role of molecular structure in enhancing UV downconverter film performance.



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Optimization of biomass-derived activated charcoal supporting TiO_2 nanoparticles as a potential photocatalyst

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Introduction

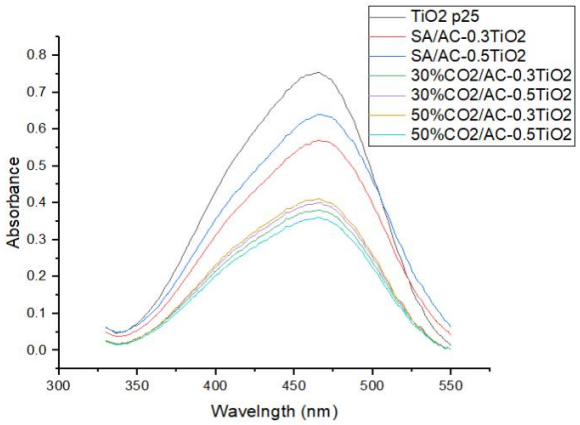
TiO_2 is a widely recognized photocatalyst[1]. However, the photocatalytic performance of TiO_2 is constrained by its low surface area, wide band gap, and high electron-hole pair recombination rates[2]. The primary aim of this study was to optimize the photocatalytic efficiency of TiO_2 by impregnating it onto activated charcoal derived from *Senegalia mellifera* biomass.[3]

Materials and Methods

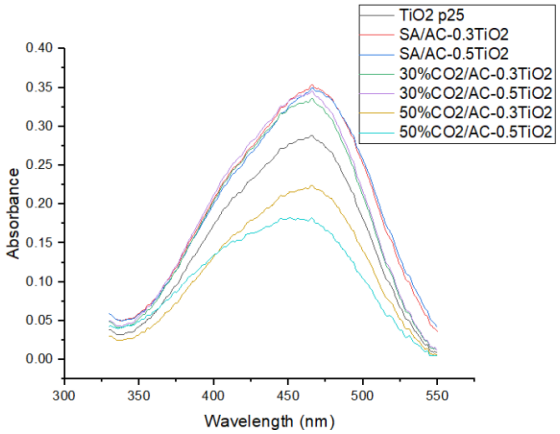
The research employed a quantitative approach. TiO_2 was synthesized using the precipitation process[4]. Bush biomass samples were collected using selective sampling. Activated charcoal was synthesized using both chemical and physical activation techniques. The as-prepared activated charcoal samples were impregnated with TiO_2 NPs using the wet impregnation method.[4]

Results and Discussion

This study aimed to optimize the effectiveness of biomass-derived activated charcoal supporting TiO_2 NPs as a potential photocatalyst for the production of green hydrogen. The objective was to address the limitations of TiO_2, particularly its low photocatalytic efficiency caused by a wide band gap, low surface area and high electron-hole recombination rates. By incorporating TiO_2 NPs onto activated charcoal synthesized from the biomass of the invasive *Senegalia mellifera* bush, this research pursued a sustainable and efficient solution to enhance TiO_2's photocatalytic activity.



Under Visible Light (Methyl Orange)



Under UV light (Methyl Orange)

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Activated Carbon from Waste Paper for The Removal of Contaminants from Wastewater

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Introduction

Water pollution is one of the major challenges faced today due to toxic pollutants released from various industries into the environment, which can be detrimental to humans and the environment[1,2]. Among various technologies used in the removal of these toxins from water, the use of activated carbon (AC) as the adsorbent is by far the most promising and economical approach because of its high adsorption capacity[3].

Materials and Methods

Activated carbon was produced from waste photocopy paper through physical and chemical activation, using 5% phosphoric acid as the impregnating agent. The paper was first de-inked via flotation with 1% sodium hydroxide, 1% sodium silicate, and oleic acid[4]. The de-inked material was then converted into activated carbon at 600 °C for 2 hours in the muffle furnace[5]. The ACs were evaluated for their effectiveness in treating contaminated water samples, including methylene blue dye, methyl orange dye, copper sulfate, and domestic wastewater.

Results and Discussion

The activated carbon (AC) derived from waste paper showed high removal efficiency for contaminants, with specific results indicating 96% removal of methylene blue dye, 94% removal of methyl orange dye, and 56% removal of copper sulphate ions. The findings further indicated that parameters such as temperature, contact time, and AC dosage had a significant effect on the removal efficiency. For instance, higher temperatures and longer contact times improved the adsorption capacity for MB and MO. At an optimal dosage of 0.1 g of AC per 100 mL of solution, the activated carbon effectively treated domestic wastewater, demonstrating reductions in turbidity by 96% and conductivity by 61%. These values affirm the potential of waste paper-derived AC as an efficient, eco-friendly adsorbent for wastewater treatment applications.

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DFT Modelling of Carbon Supported Platinum-Based Electrocatalysts

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Introduction

Thin film electrocatalysts can reduce the use of costly metals like platinum (Pt) in industrial applications[1] such as the hybrid sulphur (HyS) cycle for hydrogen production[2]. Glassy carbon (GC) is an ideal substrate due to its chemical resistance, conductivity, and thermal stability but suffers from poor metal adhesion.[3] Studies show that adding palladium (Pd) to form a bimetallic catalyst improves adhesion without sacrificing performance, though delamination still occurs, affecting durability.[4] Quantifying adhesion remains challenging, as traditional techniques are insufficient, and computational methods have yet to address GC's complex structure.

Materials and Methods

This study developed three density functional theory (DFT) models to address gaps in understanding adhesion mechanisms. The first model, a defect-induced glassy carbon (DI-GC) model, simulated GC by introducing single-point defects into an $R\bar{3}m$ carbon allotrope and validating it against published data. The second model used solid-state molecular modelling (CASTEP and GULP) to create bimetallic Pt_xPd_y catalysts (Pt_3Pd_2 and Pt_2Pd_3), analysing their atomic structure and electronic properties. The third model combined these to investigate interfacial bonding, quantifying and describing adhesion between bimetallic catalysts and GC substrates.

Results and Discussion

The models showed that Pt_3Pd_2 and Pt_2Pd_3 adhere better to DI-GC due to enhanced electron transfer and stronger interfacial interactions at defect sites. Pd atoms above defects sank into GC vacancies, further improving adhesion. Pt_3Pd_2 exhibited the best adhesion, with a work of adhesion of 2.923 J/m², electron transfer of 3.87 e^-, and a d-band shift of 0.1806 eV. These results highlight the role of interfacial defect engineering in optimising bimetallic catalysts for improved adhesion.

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Metal-organic framework modified carbon nanotubes for hydrogen production from formic acid

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Introduction

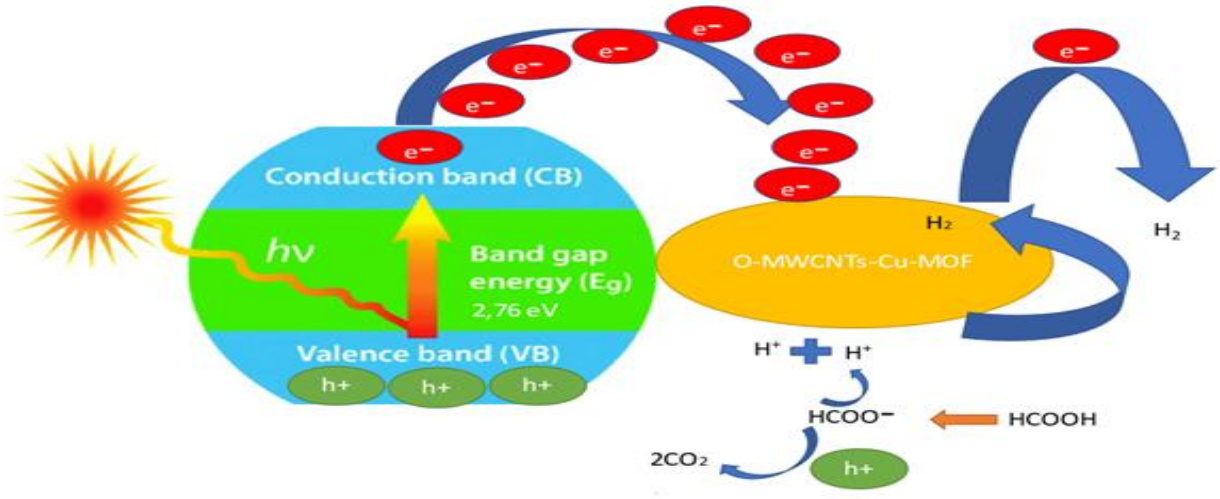
The growing global demand for sustainable energy sources and the urgent need to mitigate the impacts of carbon emissions have stimulated significant research efforts in developing novel materials for clean energy generation and carbon capture.[1] In this context, metal-organic frameworks (MOFs) and carbon nanotubes (CNTs) have emerged as promising materials for clean hydrogen production.[2] Thus, this research study introduces the first reveal of Cu-MOF integrated with CNTs as a new photocatalyst for hydrogen production with carbon dioxide capture and conversion.

Materials and Methods

The structural, thermal, and morphological characteristics of the as-prepared composite were determined using the appropriate analytical techniques, such as FTIR, XRD, and TGA. Gas chromatography was used to test the amount and purity of the gas produced.

Results and Discussion

The gas produced was recorded to be 11 mmol/g with 75% pure hydrogen. The catalyst holds the potential to be used in industrial hydrogen production because it is easy to manufacture from recyclable products.



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Removal of Contaminants from Wastewater with Activated Carbon from *Acacia Erioloba* Seed-Pods

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Introduction

Water pollution has been an ecological concern in the past few years (1,2) and it tends to be one of the contributing factors for low access to hygienic drinking water in developing countries (3). As a consequence, several methods have been explored to get rid of contaminants from water (4). The adsorption method appeared to be the best in terms of effectiveness. The current study aimed at preparing activated carbon (AC) from *Acacia erioloba* seed pods using an 5% H_2SO_4-5 % H_3PO_4 activator combination and to evaluate the efficiency of activated carbon for the removal of contaminants in wastewater.

Materials and Methods

Scanning Electron Microscopy, FT-IR spectrophotometer was used determine the morphology and the functional groups of the newly prepared activated carbon, respectively. UV-vis spectrophotometer was used to determine the concentration difference between the treated and untreated water samples.

Results and Discussion

A microporous and mesoporous activated carbon with high fixed carbon content (82.7-91.1%) and a high surface area of 411.76 m^2/g, 585.45 m^2/g, 548.69 m^2/g, for AC 1,2 and 3 respectively, was prepared which contains high oxygen surface functional groups important for adsorption. The activated carbon prepared from *acacia erioloba* seedpods can be used to treat cationic and anionic dye-contaminated industrial wastewater and to remove organic compounds from domestic wastewater. Its surface was bound with trace elements such as Mg,P,Ca, K, and Cl which infer its ability to adsorb heavy metals through ion exchange (5).

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GH_2-based ammonia-derived fertilizers, their application in desert soil fertility at Daures Village

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Introduction

Namibia's agricultural potential remains largely untapped, despite possessing vast stretches of arable land such as the Namib desert due to factors such as low soil fertility (mainly gypcrete/calcrete soil type) and water shortage[1,2]. As a result, the country finds itself compelled to import a substantial portion of its food requirements to meet the demands of its population[3]. With green hydrogen (GH_2) at the center stage in Namibia, green ammonia derived from GH_2 presents an opportunity for application in the production of smart fertilizers to improve soil fertility at Daures Village, Namib Desert, Namibia.

Materials and Methods

The research employed a quantitative approach. Liquid ammonia (NH_4OH) generated and collected from the H_2 plant at Daures village was used to produce ammonium salts (NH_4NO_3, NH_4SO_4), which were processed further and applied to the sand collected from Daures village. Other soil parameters such as pH, soil type, moisture contents, alkalinity, salinity, etc. were established, before and after the treatment[1,2]. A variety of crops were seeded and planted in the treated and untreated samples, results were compared.

Results and Discussion

The results proved that neutralizing alkalinity and adjusting salinity of the course-structured sand soil was key to have crops germinating. In addition, the addition of organic matters in the form of dry grass or others such as peals of fruits (after seeds were removed) provide much needed anchor for crops to germinate easily[4]. Transplanting trees has been recommended for the long-term sustainability smart agriculture to regulate temperature, however, in the short-term shade nets are feasible to protect crops from direct sun[5]. Thus, tomatoes and cabbages were successfully seeded, grown and sown after 3 months in the treated soil, compared to nothing in the untreated control sample. Conclusively, GH_2 application can be applied towards producing smart fertilizer for enhancing soil fertility for crop growth in areas of need including the Namib Desert.

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