Abstract: Science and Engineering Fair of Houston

3173

A Comparative Analysis of Tensile Strength and Water Absorption Between Natural Crosslinkers in Bioplastics

Andrea Shi

Conroe ISD /AST: Academy of Science and Technology

Category:

Chemistry

Increasingly, plastic pollution has become one of the most dramatic environmental issues that humanity faces, ending up in oceans and food through microplastics due to the inability of plastic to degrade naturally. An alternative suggested to address this problem is bioplastics, minimizing the risk of buildup and microplastic contamination. However, current obstacles towards the commercialization of bioplastics include their expensive production process and the fact that, without additional modifications (crosslinkers), starch-based bioplastics are at risk of structural weaknesses in terms of water absorption and tensile strength. The purpose of the experiment was to test which natural crosslinker agent (citric, ascorbic, or tannic acid) produces the most substantial starch-based bioplastic in terms of water-absorption rate and tensile strength to mimic petroleum-plastics. It was hypothesized based on previous research that tannic acid would be the optimal crosslinker agent. The study followed three main phases: sample creation, water absorption testing, and tensile strength testing. Five trials were conducted per crosslinker type (citric, ascorbic, tannic, and a control group) for each type of test. One-way ANOVA tests were performed to calculate the significant difference between both average water absorption rate and tensile strength across the four groups (4.37×10^{-21} and 1.31×10^{-13}, respectively). As predicted, tannic acid was the most optimal crosslinker agent. The application of this study was to further the development of bioplastics in an inexpensive manner using natural crosslinking agents in order to produce a realistically market-feasible product for future commercialization.

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[ ] Vertebrate animals [ ] microorganisms [ ] rDNA [ ] tissue

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Abstract: Science and Engineering Fair of Houston

3174

Food preservatives

Grace Romano

Pasadena ISD/Pasadena Memorial High School

Category:

Chemistry

The purpose of this experiment is to bring awareness that people with limited financial resources tend to rely on cheaper accessible fast-food sources around them locally but may, or do not know how diets consisting only processed meals can be unhealthy and harmful due to their chemical preservatives and lack of nutrition provided. Additionally, also potentially highlighting issues on the cost of fresh produce which influences the meals they eat as well. My hypothesis was, "If chicken nuggets are highly processed then they will show little or no mold growth in an extended period of time." To perform this experiment, I will be preparing homemade chicken nuggets and retrieving, both McDonald's chicken nuggets & Chick-fil-A's grilled chicken nuggets, in order to compare all three their process of decomposition so then I can take notes on whether there are different condensation sightings, discoloration patterns, weight, temperature, and when mold/bacteria growth shows. I believe after conducting my experiment the results will show that, yes, chicken nuggets which are highly processed will show little or no mold growth in an extended period of time because they've been made to last longer and have unfavorable/unhabitable environments for bacteria development where a growing population needs faster food production w/ limited resources.

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Abstract: Science and Engineering Fair of Houston

3175

Category: Chemistry

Utilizing Grand Canonical Monte Carlo Simulations to Identify Optimal Zeolites in Post-combustion Carbon Capture

John Lezama

Tomball ISD/Tomball HS

Anthropogenic carbon dioxide (CO2) emissions are the primary contributor to rising global temperatures. Post-combustion carbon capture (PCC) filters CO2 from factory exhaust before it enters the atmosphere, significantly reducing emissions. However, PCC's high costs hinder its implementation and thus its impact in reducing emissions. Zeolites are alumino-silicate crystals that serve as filters in PCC, possessing a silicon-to-aluminum ratio (Si/Al) that affects their performance. Na-FAU and Na-LTA are considered industry-standard zeolites for PCC; however, of the over 250 zeolites, fewer than half have been evaluated for carbon capture. This study addresses this research gap and searches nine zeolites across nine Si/Al ratios, including configurations that have not been tested in previous literature, to determine if industry standards could be outperformed. As a result, previously unexplored Na-RWY with a Si/Al of 1.0 was simulated to outperform Na-FAU by 143% and 191% and Na-LTA by 154% and 387% in adsorption capacity and working capacity, respectively. Additionally, the accessible volume of zeolite frameworks strongly correlated with adsorption and working capacity (R = 0.94 and R = 0.98, respectively), providing a structural explanation and backing for simulated results. Although only nine frameworks were tested and physical experimentation is required to confirm the validity of results, the discovery of Na-RWY could shift industry benchmarks, highlighting the potential of future testing of overlooked zeolites to lower costs and encourage widespread adoption of carbon capture.

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Abstract: Science and Engineering Fair of Houston

3176

The Effectiveness of Eco-Friendly vs. Commercial Cleaning Products

Grace Enobie, Jaqueline Ramos

Alief ISD/Hastings HS

Category:

Chemistry

This experiment comparing the effectiveness of a commercial stain remover (Shout) and Eco-friendly cleaner (baking soda and vinegar) in removing coffee, ketchup, and orange juice from cotton (C), polyester (PES), and polypropylene (PP). Each fabric sample measured 21 x 28 cm, and each stain used the same amount of liquid: 1 teaspoon of coffee, 1 teaspoon of ketchup, and 1 tsp of orange juice. Cotton absorbed stain the fastest, PES absorbed moderately, and PP barely absorbed any stains. After blotting, each stain was treated with Shout and the Eco-friendly cleaner. Overall, Shout removed all stains more quickly and successfully, especially coffee and ketchup. Eco-friendly cleaners lightened stain but never removed them completely. Result supported the hypothesis that the commercial cleaner would perform best.

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Abstract: Science and Engineering Fair of Houston

3177

Iodine Clock Reaction

Category:

Chemistry

Hazel Stubbert, Anavi Shelare, valeria chapa

Fort Bend ISD /Hightower High School

This experiment has been used as a student demonstration for decades. It allows students a beginner's view on chemical kinetics. This and similar experimentation has led to many discoveries in chemical kinetics. Multiple universities and accredited chemistry institutions have written on this. How can the concentration of a substance change reaction time? The purpose of this experiment was to help demonstrate the importance of measurements and chemical kinetics. Based on our research, we predicted the substances with higher concentrations would react faster.

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Abstract: Science and Engineering Fair of Houston

3178

Category:

Chemistry

Effects of Sugar Substitutes on Amylase Activity in Starch Digestion Using an Iodine-Starch Assay

Miley Huynh

Clear Creek ISD /Clear Lake High School

Consumers increasingly rely on artificial and alternative sweeteners despite the poor understanding on the full effects that artificial sweeteners have on the body. This study investigated how six common sugar substitutes (aspartame, sucralose, monk fruit, stevia, sorbitol, and erythritol) affect the rate at which amylase breaks down starch using an in vitro iodine-starch assay. A 1% cornstarch solution was combined with individual sugar solutions and exposed to a 0.05 g/100 mL amylase mixture at 37°C. Samples were taken every 30 seconds for 10 minutes, mixed with Lugol's iodine, and analyzed by color intensity, where faster fading indicated greater starch breakdown and higher amylase efficiency. All tested sweeteners reduced amylase activity to some degree, but the extent of inhibition varied by sweetener type. Aspartame produced the slowest rate of color change across all concentrations, indicating the strongest inhibition of amylase function. In contrast, the naturally derived sweeteners monk fruit and stevia showed only mild inhibition, especially in lower concentrations. Sorbitol and erythritol (sugar alcohols) showed greater inhibition than the novel sweeteners, but less than the artificial sweeteners. Overall, the results demonstrate that aspartame most significantly slows starch digestion by amylase, while monk fruit and stevia have the least impact.

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Abstract: Science and Engineering Fair of Houston

3179

Fruit Nutritional Value

Temiloluwa Ogunlaja, Candy Hernandez

Fort Bend ISD /Hightower High School

Category:

Chemistry

This project examines the vitamin C levels in various types of fruits. We used a chemical mix of DCPIP with our fruit concentrate. The purpose of this experiment was to determine how much vitamin C is actually in the fruit we eat. Vitamin C is a vital nutrient that supports the human body's health. We used the technique of titration. The slowly dripping DCPIP into the vitamin C solution, until a color change happens. We repeated the steps with our apples, oranges, and grape concentrate. All testing was done in a controlled laboratory with proper safety measures. In conclusion, the experiment demonstrated how chemistry can be applied to real-life activities.

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Abstract: Science and Engineering Fair of Houston

3180

Moisture Retention

Sumaiyya Mushtaq, Jana Bader, Maryam Sayed

Private/Houston Quran Academy - Spring HS

Category:

Chemistry

Our topic is about moisture retention in different moisturizers. We wanted to identify which moisturizer to use when in need of the most moisture retention. We think the La Roche-Posay moisturizer would hold the most moisture. We used petri dishes with Jell-O as skin models, with the control group receiving no moisturizer. The mass of each dish was recorded every day for ten days.

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Abstract: Science and Engineering Fair of Houston

3181

Category:

Chemistry

Controlling Drug Release from Alginate Hydrogel Beads Using Polymer Coatings

Madeleine Melancon

Houston ISD/Carnegie Vanguard HS

Controlled drug delivery systems can improve chemotherapy effectiveness while reducing side effects. This study investigated how pH and polymer coatings affect the release of doxorubicin from calcium–alginate beads. Beads were prepared with sodium alginate and calcium chloride, then left uncoated or coated with chitosan, polyethyleneimine (PEI), or a combination of PEI and polyacrylamide (PAA). Drug release was tested in citrate buffer (pH 5), phosphate-buffered saline (PBS, pH 7), and Tris buffer (pH 9). Uncoated beads released about 75% of doxorubicin within 4 hours at all pH levels, with the fastest release at pH 9 and slowest at pH 5. Polymer coatings slowed release across all pH values, with chitosan+alginate most effective at pH 5, PEI+alginate at pH 7, and PEI+PAA at pH 9. These results show that polymer-coated alginate beads provide pH-dependent, controlled drug release, demonstrating their potential for targeted chemotherapy and reduced harm to healthy cells.

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Abstract: Science and Engineering Fair of Houston

3182

Category:

Chemistry

Enhancing Charcoal Adsorption with Acid and Base Treatments to Capture Microplastics

Diya Pillai

Conroe ISD /AST: Academy of Science and Technology

Microplastic pollution has emerged as a significant environmental concern, with particles smaller than 10 micrometers increasingly detected in natural water systems and drinking water sources. Due to their small size and persistence, microplastics are difficult to remove using conventional water treatment methods, creating a need for low-cost and effective filtration alternatives. This study investigates whether simple chemical surface treatments can enhance the ability of charcoal to adsorb microplastics from water. Charcoal samples were treated using phosphoric acid (H_3PO_4) and sodium bicarbonate ($NaHCO_3$) at concentrations of 0.1 M, 0.3 M, and 0.5 M, alongside untreated charcoal as a control. Treated and untreated samples were exposed to water contaminated with 5 µm polystyrene microbeads under controlled laboratory conditions. Following filtration, remaining microplastic concentrations were quantified using a PASCO spectrometer by measuring light absorbance caused by particle scattering. Results showed that phosphoric acid–treated charcoal significantly improved microplastic removal, with the 0.5 M acid treatment achieving a maximum removal efficiency of approximately 86%. In contrast, sodium bicarbonate treatment reduced adsorption efficiency, with removal rates decreasing below the untreated control as concentration increased. These findings suggest that acid activation enhances charcoal microporosity and surface functionality, while base treatment may introduce electrostatic repulsion. Overall, this study demonstrates that acid-treated charcoal offers a low-cost, scalable, and sustainable approach for reducing microplastic contamination in water systems.

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Abstract: Science and Engineering Fair of Houston

3183

Sticky Solutions vs. the world

Kayla Cox

Clear Creek ISD /Clear Springs High School

Category:

Chemistry

The purpose of this experiment was to see if the homemade glue I made worked better than brand glue you would find in stores. This project was to try to see if glue made from household materials would do better than brand glue. This project helped determine which glue was the stickiest. Using different glues and multiple 5 x 5 squares of cardstock, I was able to determine which glue was the best to use. I learned that Aleene's glue was the stickiest with the average height it opened was Aleene's glue at 11/48 inches, while the homemade glue was the worst with the average height opened was 37/12 inches. I learned that Aleen's glue was the best to use, and the homemade glue was the worst to use, based on how much it stuck to the paper. If I were to do this project again, I would try the original mixture of homemade glue with flour instead of cornstarch, and I would try to spread the glue on the paper a little more evenly. n.

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Abstract: Science and Engineering Fair of Houston

3184

Category:

Chemistry

Structure-Based Virtual Screening and Computational Characterization of SIRT7 as a Therapeutic Target in Small Cell Lung Cancer

Srinidhi Kolachalam

Fort Bend ISD /Dulles High School

Small cell lung cancer (SCLC) is an aggressive and rapidly progressing form of lung cancer with limited treatment options and poor survival rates. SIRT7 is an enzyme that regulates tumor growth and has been implicated in promoting the aggressiveness of SCLC. Small-molecule ligands that bind effectively to the active site of SIRT7 can inhibit its function, thereby reducing tumor progression and aggressiveness in SCLC. This study aims to identify and evaluate potential small-molecule inhibitors targeting the SIRT7 protein in small cell lung cancer (SCLC) using computational molecular docking techniques. The amino acid sequence of human SIRT7 was retrieved from the UniProt database, and its three-dimensional structure was predicted using AlphaFold 3 to provide a reliable model for molecular docking. Ligands were collected from the ZINC20 database and prepared for structure-based virtual screening. Molecular docking was performed using AutoDock Vina to evaluate the binding affinity of each ligand to the SIRT7 active site. The most promising protein–ligand complexes were further assessed using PRODIGY to validate and quantify their binding energy. Additionally, the pharmaceutical properties and toxicity profiles of the top candidate were evaluated through the ADMET AI webserver to predict drug-likeness and safety. From this integrated computational analysis, ligand IV emerged as the most promising inhibitor, exhibiting the most negative binding energy of -5.30 kcal/mol and demonstrating favorable ADMET properties. These findings support the hypothesis that small-molecule ligands capable of effectively binding to the SIRT7 active site can suppress its function and may reduce SCLC progression. The current research will help in designing novel treatment targeting small cell lung cancer and provides a computational framework for developing SIRT7 inhibitors that can be validated in future experimental studies.

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Abstract: Science and Engineering Fair of Houston

3185

How does carbon nanopowder improve sodium ion uptake in Coriandrum sativum?

Katherine Liu, Aimee Wang

Conroe ISD /AST: Academy of Science and Technology

Category:

Chemistry

Soil salinity is a major global agricultural challenge, affecting approximately 10% of the world's land area and significantly reducing crop growth and yield by disrupting nutrient uptake, osmotic balance, and enzyme activity in plants. Traditional mitigation methods, such as biochar application, help reduce salinity effects indirectly by improving soil structure and binding sodium ions, but their effectiveness is limited. This study investigated whether carbon based nanoparticles could more effectively improve plant tolerance to saline conditions compared to biochar. Coriandrum sativum, or cilantro, was grown in four treatments including control (salinized soil), no salinization, biochar, and carbon nanoparticles. Soil was artificially salinized using a sodium chloride solution, and plant growth was monitored over six weeks by measuring germination rate, plant height, and soil electrical conductivity. Results showed that plants grown without salinity had the highest overall growth. However, among salinized treatments, the carbon nanoparticle group exhibited taller plants, higher germination rates, and the greatest reduction in soil salinity compared to both the biochar and control groups. In contrast, soil salinity increased over time in the control group. These findings support the hypothesis that carbon nanoparticles enhance plant tolerance to saline conditions more effectively than biochar. This research suggests that carbon nanoparticles have potential as a sustainable and cost effective soil amendment for improving crop growth in saline soils, contributing to agricultural productivity, soil remediation, and global food security.

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Abstract: Science and Engineering Fair of Houston

3186

Computational Discovery of Key Active Components in Antimalarial Drugs

Ksenia Kolomeisky

Houston ISD/Carnegie Vanguard HS

Category:

Chemistry

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Abstract: Science and Engineering Fair of Houston

3187

Category: Chemistry

UricA! In Silico Screening to In Vitro Validation of Xanthine Oxidase Inhibitors

Riya Singhal

Tomball ISD/Tomball Memorial - HS

Hyperuricemia and gout are rising metabolic disorders, highlighting the need for safer, more effective therapies. Xanthine oxidase (XO), a pivotal enzyme in uric acid synthesis, is the prime therapeutic target; however, current inhibitors - allopurinol, febuxostat, and topiroxostat - remain constrained by adverse effects and suboptimal access to the deeply embedded molybdenum-pterin (Mo-Pt) catalytic site of the enzyme. This study employed a dual-stage pipeline combining computational and experimental innovation to discover novel XO inhibitors. Virtual screening and ADMET analysis of inhibitor-bound XO crystallography identified unexpected lead candidates, with structural clustering prioritizing vitamin B analogues (folic acid, niacinamide, nicotinic acid) and botanicals (Moringa oleifera, Curcuma longa, Zingiber officinale) for further evaluation. Experimental in vitro assays reaffirmed allopurinol as the performance standard. Dual-agent combinations, especially those including allopurinol, delivered the highest and most sustained inhibition across all concentrations. Notably, the combination of folic acid and moringa showed peak efficacy among non-synthetics, sustaining potent, dose-dependent inhibition even at higher dilutions. Although Kruskal-Wallis testing did not reach statistical significance, rank-based analysis consistently revealed biologically meaningful efficacy trends and robust combination effects. These findings support a tiered, personalized approach based on disease severity: folic acid or moringa extract for mild cases; synergistic regimens combining low-dose allopurinol with either folic acid or moringa for moderate disease; and allopurinol plus moringa for severe gout. This study advances an integrative chemistry-pharmacology approach, bridging computational prediction with experimental validation and paving the way for next-generation xanthine oxidase inhibitor therapies to address key unmet clinical needs in gout and hyperuricemia management.

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Abstract: Science and Engineering Fair of Houston

3188

Silicon–Carbon Composite and P-Type Silicon Anodes for Sodium-Ion Batteries

Aditya Kejriwal

Private/The Kinkaid School - HS

Category:

Chemistry

Sodium-ion batteries are being researched as a low-cost and sustainable alternative to lithium-ion batteries. However, as cell design is being developed, there are questions about efficient electrode and electrolyte materials. Currently, carbon-based compounds are the leading anode material, but silicon's high specific capacity makes it efficient and its abundance in the crust makes it economically and environmentally ideal. This study employed atomistic simulations to research the use of silicon as sodium-ion battery anode material. Using the Atomic Simulation Environment (ASE) a carbon coated silicon sphere, layered silicon-graphite composite, and p-type silicon was modeled. Molecular Dynamics simulations were performed at 300 K with a 1fs timestep to simulate sodium insertion and removal over multiple charge cycles, assessing structural stability and volumetric changes. Conductivity was estimated using BoltzTraP2. It was found that introducing carbon to the silicon structural greatly increased stability and decreased breakage while doping with boron had minimal effects. However, both methods did increase the conductivity. These findings suggest that carbon-silicon composites could be a potential sodium-ion battery anode material and further research should be done to find the optimal carbon to silicon ratio and structure.

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Abstract: Science and Engineering Fair of Houston

3189

Category:

Chemistry

Advancing Applications of AI Predictive Models by Experimental Validation in Saltwater Battery Performance

Ronit Chheda

Fort Bend ISD /Clements High School

Surging power demand from AI data centers has led to growing sustainability challenges. Direct use of non-renewable energy sources contributes to global warming, responsible for unstable climate patterns on Earth. The plausible solution of utilizing clean energy sources has failed due to intermittency issues. Hence, a viable, large-scale energy storage system is required. Next-generation saltwater batteries are cheap, sustainable alternative to today's primitive energy storage systems. Previous work presented at SEFH, TXSEF, JIC-2024 on saltwater batteries explored various anode materials and had shown Zinc as the most promising anode material in battery performance. Hence, the current work has further investigated Zn-C battery operational parameters in the presence of different electrolytes. Moreover, effect of pH and operating temperature on battery performance was determined. Among NaCl, Na2SO4, and KCl used as different electrolytes, KCl resulted in high voltage and 5 times higher current (mA) readouts compared to the control (water). Whereas low pH environment and high operating temperature resulted in better performance compared to controls. These experimental findings corroborate with the AI predictive model presented by Cao et al. 2025 who have shown that high ZnCl2 concentration suppressed H2O-splitting side reactions, increasing conductivity and performance of Zinc-ion saltwater battery. Another AI predictive study (Zhang et al. 2023) revealed the role of electrolytes in reorienting water molecules thus improving conductivity. Taken together, experimental validation with AI predictive models improves scientific understanding in saltwater battery technology for large-scale energy storage applications that could in turn potentially provide clean power for AI data centers.

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Abstract: Science and Engineering Fair of Houston

3190

Finding the Pairfumer: Which LLM Blends Best?

Maha Sttar, Sarah Al-baidhani

Harmony Public Schools - South District/Harmony Science Academy-Houston

Category:

Chemistry

This study evaluated human perception of essential oil perfume blends generated by four large language models (LLMs) to determine whether machine learning can produce formulations preferred by human evaluators. GPT-5.2-Pro, GPT-5.2 Extended Thinking (OpenAI), Claude Opus 4.5 (Anthropic), and Gemini 3 Pro Preview (Google) were each prompted with identical instructions to generate three perfume formulas (Accessible, Distinctive, Sophisticated profiles) using a dataset of 140 reference blends and a restricted palette of 20 essential oils. The resulting 12 formulas were prepared as 10% dilutions in dipropylene glycol and presented via blotter strips in a blind evaluation protocol. Preliminary data from 10 adult participants revealed significant performance differences between LLMs. GPT-5.2-Pro achieved the highest preference scores, with its sample selected as first choice by 50% of participants (18 total points). GPT-5.2 Extended Thinking ranked second (12 points), described as "nostalgic" and "candle." Claude Opus 4.5 placed third (10 points), consistently chosen as second preference but never first. Gemini 3 Pro Preview performed poorest (5 total points), with one sample receiving zero selections. These preliminary results suggest OpenAI models outperform competitors for creative formulation tasks. Data collection is ongoing; final results with expanded sample size and statistical analysis will be reported.

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Abstract: Science and Engineering Fair of Houston

3191

Which carbon filters water best?

Category:

Chemistry

Angel Alvarez

Alief ISD/Elsik HS

This project investigated how the particle size of activated carbon affects water filtration. Activated carbon is widely used in water treatment because it removes impurities through adsorption, but different filters use different particle sizes. The purpose of this experiment was to compare granular activated carbon with crushed activated carbon to determine which type removes more color from dyed water and how particle size influences filtration speed and effectiveness. Both carbon types were tested in three trials using equal amounts of dyed tap water, and all other variables were kept constant. Filtration time was measured with a timer, and water clarity was rated using a color scale. The results showed a clear tradeoff. Granular activated carbon filtered the water much faster, averaging about 24 seconds, but removed very little dye. Crushed activated carbon filtered more slowly, averaging over 34 seconds, yet consistently produced much lighter, cleaner water. These findings support the hypothesis that smaller particles provide more surface area for adsorption, making crushed carbon more effective at removing contaminants. A fizzing effect observed in the crushed carbon trials may have contributed to the slower flow rate. Overall, the experiment demonstrated that crushed activated carbon is the better choice when cleaner water is the goal, even though it filters more slowly. This reflects real‐world filtration systems, where crushed or powdered carbon is used for deeper purification. Future improvements could include more trials, testing other contaminants, or combining both carbon types to balance speed and effectiveness. This investigation helps explain how activated carbon works and why particle size matters in modern water‐cleaning technology.

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Abstract: Science and Engineering Fair of Houston

3192

Improving Hydrogen Production: Surfactants in Alkaline Electrolyzers

Prachi Natoo

Conroe ISD /AST: Academy of Science and Technology

Category:

Chemistry

Transportation is responsible for roughly one-third of U.S. carbon dioxide emissions and the majority of petroleum consumption. While hydrogen could significantly reduce these emissions and petroleum dependence, green hydrogen remains too expensive to compete with fossil fuels. Electrolysis, the chemical process of splitting water into hydrogen and oxygen, remains one of the most promising methods for clean hydrogen production. However, issues such as electrode corrosion and bubble adhesion make alkaline electrolysis difficult. After demonstrating small-scale forced convection in electrolyzers last year, this project tested the passive forced convection in a large-scale, real-world environment. The electrolysis system was scaled up to a 66-liter model, requiring redesigns of mounts to maintain performance at higher volumes. Another major focus of this project was reducing gas bubble adhesion on electrode surfaces. In addition to forced convection, the surfactant Sodium Lauroyl Glycinate was added to the electrolyte solution to reduce surface tension and increase bubble acceleration. With the surfactants, the bubbles velocity increased by .012 meters per second, and the bubble diameter significantly decreased. Additionally, scaling up the prototype provided proportional bubble volume, as well as increased the electrode longevity, further proving this design's industrial viability. Green Hydrogen has the potential to conserve petroleum, meet increasing energy demands, and make America's energy system more resilient. This project is the first of its kind to successfully decrease bubble adhesion without external energy at a higher scale, confirming the ability of forced convection paired with surfactants to increase green hydrogen efficiency.

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Abstract: Science and Engineering Fair of Houston

3193

Category: Chemistry

Computationally Determining Active Site Behavior of Cobalt Single Atom Catalysts in the First Step of Carbon Monoxide Hydrogenation

Manas Kinge

Conroe ISD /AST: Academy of Science and Technology

This project investigated the effectiveness of Co-N2C2, Co-N4, and Co-N3C single atom catalysts (SACs) in the rate limiting CO to CHO step for CO hydrogenation. The hypothesis was Co-N2C2 and Co-N3C perform better than Co-N4. These SACs were modeled using the Avogadro 2 software, alongside with a Co-N4 catalyst poisoned with an axial sulfur as a negative control. The project used the Python Atomic Simulation Environment (ASE) and GPAW libraries to run a Density Functional Theory simulation of the cobalt SACs. First, vacuum convergence was performed to determine proper simulation space around the molecule. Then the ASE optimizer was set on Fast Inertial Relaxation Engine mode to relax the SAC structure. Adsorption energies were tested at 2 Angstroms above the active site, 1 Angstrom lateral of the active site, and 2 Angstroms lateral of the active site. After this the activation barrier was determined using a nudged elastic band with 5 total images, showing a hydrogen approaching adsorbed CO. Projected density of states was obtained by combining spin states and graphed with Matplotlib for electron state distribution. Using this, d band centers were computed. The hypothesis was proven correct, and the best catalyst was Co-N2C2 with each site adsorption energy as -1.566 eV, -1.751 eV, and -1.606 eV respectively. It had the lowest activation barrier of 0.367 eV, a moderate d-band center of -1.896 eV, and a balanced electron state distribution.

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