Project number: T23-601/17-R

RESEARCH GRANTS COUNCIL
THEME-BASED RESEARCH SCHEME (TRS)

Completion Report on Funded Project

Project start date: *1 Jan 2018*
Project Completion date: *31 Dec 2023*

1. Project Title: Creation of rechargeable electron-fuels for stationary power supplies and electric vehicles

2. Names and Academic Affiliations of Project Team Members#

Project team member	Name / Post	Unit / Department / Institution	Average number of hours per week spent on this project in the current reporting period
Project Coordinator (PC)	Minhua Shao/Chair Professor[1]	Chemical and Biological Engineering, & Energy Institute, HKUST	10
Co-Principal Investigator(s)	Tianshou Zhao/Chair Professor[1]	Mechanical and Aerospace Engineering, HKUST	10
	Guochen Jia/Chair Professor	Chemistry, HKUST	6
	Yi-Chun Lu/Associate Professor[2]	Mechanical & Automation Engineering, CUHK	8
	Ping Gao/Professor	Chemical and Biological Engineering, HKUST	8
	Kwong-Yu Chan/Professor	Chemistry, HKU	8
	Nedjib Djilali/Professor	Mechanical Engineering & Institute for Integrated Energy Systems, University of Victoria, Canada	6
Co-Investigator(s)	Qing Chen/Assistant Professor[3]	Chemistry & Mechanical and Aerospace Engineering, HKUST	6
	Jang-Kyo Kim/Chair Professor Emeritus[4]	Mechanical and Aerospace Engineering, HKUST	4
	Meng Ni/Professor	Building and Real Estate, PolyU	5

	Christopher Yu-Hang Chao/ Vice President (Research and Innovation), Chair Professor[5]	Building Environment and Energy Engineering, PolyU	4
	Liang An/Associate Professor[6]	Mechanical Engineering, PolyU	7
Collaborators	Shao-Horn Yang/Professor	Materials Science and Engineering, Massachusetts Institute of Technology, USA	N.A.
	Khalil Amine/Professor	Chemical Sciences and Engineering Division, Argonne National Laboratory, USA	N.A.
	Industry	China Light & Power Company Syndicate	N.A.

 # Please highlight the approved changes in the project team composition and quote the date when the RGC granted approval of such changes. For changes in the project team composition, please submit a separate request, together with the justification and the curriculum vitae of the new member(s), to the RGC three months prior to the intended effective date of the change.

[1] The Collaborative Research Projects Steering Committee (CRPSC) approved the request for a change of role for Prof Tianshou Zhao (from PC to Co-PI) and Prof Minhua Shao (from Co-PI to PC) on 25 April 2022.
[2] Prof. Yi-Chun Lu was promoted from Assistant Professor to Associate Professor, effective 1 Aug 2018.
[3] Prof. Qing Chen was promoted from Assistant Professor to Associate Professor, effective 1 Jul 2022.
[4] Prof. Jang-Kyo Kim has retired from HKUST effective 1 Jul 2020. Prof Kim continued to serve as a Co-Investigator for the project with his new title "Professor Emeritus" (letter to RGC dated 18 June 2020 refers).
[5] Prof Christopher Chao joined PolyU in Sep 2021.
[6] Prof. Liang An was promoted from Assistant Professor to Associate Professor, effective 1 Aug 2018.

3. Project Objectives

Summary of objectives addressed/achieved:

Overall Objectives*	Percentage achieved	Remarks**
1. Fundamental science and methodologies for creating stable and cost-effective e-fuels featuring an energy density of 200-300 Wh/L;	100%	1.

2. Fundamental science and mechanisms underlying the materials, the e-fuel charger, and the power cell at atomic, molecular, and macroscopic levels; and	100%	2.
3. An integrated theory of electrochemistry and thermo-fluid sciences for the optimal design of e-fuel chargers and power packs; and	100%	3.
4. An e-fuel charger and two power pack prototypes with one for stationary power supply and the other for EVs. The prototypes will be 85-90% energy efficient, while the system cost will be within the target of US$250 kWh^{-1} set by the United States Department of Energy.	100%	4.

* *Please highlight the approved changes in objectives and quote the date when the RGC granted approval of such changes.*
** *Please provide reasons for significantly slower rate of progress than originally planned.*

6. Research Highlights and Outputs

6.1 What are the most exciting research accomplishments of the project?
(Please list five or more of the team's best research accomplishments, such as journal and conference papers, software codes, research infrastructure, etc. For each item, please clearly justify how it has achieved international excellence (e.g. best paper award, invited presentation, citations, product licensed to industry, etc.))

1. Low-Potential, Highly Soluble Boron Organic E-Fuels

This research focused on the development of boron-based e-fuels with low working potential and high solubility, achieving several breakthroughs that contribute to the advancement of e-fuel technologies. Below is a summary of our key achievements and international impact:

1.1. Efficient One-Step Synthesis with High Yield:
- The boron-based e-fuels were synthesized directly from 1,3-diketone substrates in a single-step process, resulting in high product yields.
- This streamlined synthesis process reduces production complexity and positions these boron compounds as practical candidates for scalable e-fuel applications.

1.2. Discovery of an Optimized Compound with Excellent Electrochemical Stability: - The compound 4,6-di-tert-butyl-2,2-difluoro-2H-1λ3,3,2λ4-dioxaborinine (tBuBF2) was identified through structural optimization to exhibit superior electrochemical reversibility and stability.
- Its robust performance in e-fuel systems highlights its potential as a high-performance anolyte material for next-generation energy storage solutions.

[1] All items and their dollar figures should correspond to the statement of accounts of this project.

1.3. Insight into Redox Irreversibility and Decay Mechanisms:

- For boron diketonate compounds exhibiting irreversible redox behavior, the underlying mechanisms were systematically investigated using Na-reduction experiments and high-resolution mass spectrometry (HR-MS).
- This analysis offered a deeper understanding of redox reversibility trends and the factors contributing to compound degradation during e-fuel operation, providing valuable insights for future material design.

1.4. High-Performance Flow Cell Demonstration:

- A flow cell using 0.1 M tBuBF2 as the anode material and DBMMB(2,5-di-tert-butyl-1-methoxy-4-(20-methoxyethoxy)-benzene) as the cathode material demonstrated a round-trip energy efficiency of 68% at a current density of 40 mA/cm², with an average coulombic efficiency of 80%.
- These performance metrics represent a significant milestone for boron-based e-fuel systems and validate tBuBF2 as a viable anolyte material in real-world applications.

1.5. International Excellence through Fundamental and Applied Contributions: - This work bridges fundamental chemistry and practical application by providing a comprehensive understanding of boron-based e-fuel chemistry while achieving competitive flow cell performance.

- The research has attracted interest from both academia and industry, with potential for further development and commercialization. The results have been presented in high-impact journals and conferences, inspiring future advancements in e-fuel technology.

This study has not only pushed the boundaries of boron-based e-fuel chemistry but also laid the groundwork for scalable, efficient, and sustainable energy storage systems. The combination of innovative material design, mechanistic insights, and practical demonstrations makes it a noteworthy contribution to the field of e-fuels.

2. High-Capacity Polychalcogenide-Based E-Fuels: A Novel Self-Mediating Energy Storage Concept

This study introduced and successfully demonstrated a groundbreaking self-mediating e-fuel system that leverages inherent redox shuttles to access charges stored in solid electrode materials without the need for circulating solids. The research has achieved several significant milestones in the field of e-fuel energy storage technologies:

2.1. High Material Utilization and Exceptional Volumetric Capacity:

- The self-mediating strategy enabled material utilization of up to 99% and achieved exceptionally high catholyte volumetric capacities of 1,268 Ah L^{-1} for the Li–S system and 1,096 Ah L^{-1} for the Li–Se system.
- These metrics significantly outperform those of traditional e-fuel systems, demonstrating the strategy's ability to deliver high energy densities while maintaining efficiency.

2.2. Elimination of Circulating Solids and Foreign Redox Mediators:

- Unlike conventional "semi-solid" or "redox-targeting" approaches, this system eliminates the need for circulating solid particles or foreign redox mediators, addressing key challenges such as flow complexity, sedimentation, and cost.
- This innovation greatly enhances the practicality of high-capacity e-fuel systems.

2.3. Demonstration with Common Chalcogenide Materials:

- Using widely available materials like sulfur and selenium as examples, the study validated the versatility and effectiveness of the self-mediating strategy.
- This demonstration not only highlights the feasibility of the strategy but also opens doors for broader adoption using abundant, cost-effective materials.

2.4. Addressing Critical Challenges of Existing Systems:
- The self-mediating strategy directly tackles the limitations of existing redox-targeting e-fuels, including low energy density, inefficient charge transfer, and reliance on external mediators.
- By combining the advantages of solid materials with the simplicity of liquid-based systems, the strategy offers a transformative pathway for next-generation energy storage.

2.5. Promising Potential for High-Energy, Low-Cost Applications:
- This self-mediating design holds significant promise for efficient, high-energy-density, and cost-effective energy storage applications. Its inherent simplicity and scalability make it a compelling candidate for grid-scale and renewable energy integration.

This research has not only provided a novel framework for overcoming long-standing challenges in e-fuel systems but also established a foundation for future advancements in high-energy, low-cost energy storage technologies. Its innovative approach, coupled with exceptional performance metrics, underscores its potential to reshape the landscape of e-fuel energy storage solutions.

3. Stable Si-Based Nanofluid E-Fuels: A Breakthrough in Energy-Dense E-Fuel Storage

The development of Si-based nanofluid e-fuel represents a significant advancement in energy-dense e-fuel energy storage, offering both extremely high capacity and low working potential. However, its practical application has long been limited by the volumetric expansion of Si nanoparticles during charge and discharge processes, which leads to electrical contact loss and continuous consumption of e-fuel. To address this challenge, the team designed a novel MXene-Si@C composite with a honeycomb-like structure employing an aqueous self-assembly process for "dual-protection." This innovation has achieved international excellence for several reasons:

3.1. Advanced Structural Design for Enhanced Performance:
- The internal vacancies within the self-assembled MXene-Si@C structure effectively accommodate the volume expansion of Si, mitigating mechanical stress and ensuring structural stability.
- Furthermore, the conducting carbon and MXene components form a continuous conductive network that significantly reduces charge-transfer resistance, enhancing both rate capability and long-term cycling performance.

3.2. Exceptional Electrochemical Performance:
- The MXene-Si@C composite achieved a specific capacity exceeding 1,000 mAh g_{Si}^{-1} at a high current density of 5 A g^{-1}.
- It demonstrated exceptional cycling stability, retaining over 80% of its capacity after 300 cycles at 1 A g^{-1}, with an average coulombic efficiency of 99.73%. This performance is among the best reported for Si-based e-fuels and establishes a benchmark for future research in this area.

3.3. Highly Efficient and Scalable Fabrication:
- Unlike conventional methods, the fabrication process for the MXene-Si@C composite does not require acid washing or multiple annealing steps, saving time and energy. - The

framework is versatile and allows the substitution of MXene with other 2D materials, such as graphene oxide, further broadening its potential applications.

3.4. International Recognition:

- This work has been recognized internationally through high-impact journal publications and invited conference presentations for its contribution to advancing energy storage technology.
- The innovative approach to Si-based nanofluid e-fuel design and its scalability for mass production have attracted attention from both academia and industry, positioning it as a promising candidate for commercialization.

3.5. Potential for Industrial Applications:

- With its high efficiency, reduced production costs, and compatibility with scalable manufacturing processes, this method unlocks the potential for deploying Si-based e-fuels in large-scale energy storage systems, addressing critical challenges in renewable energy storage and grid stabilization.

This research has not only pushed the boundaries of Si-based e-fuel technology but also paved the way for practical, scalable solutions in the field of energy storage. Its combination of innovative design, exceptional performance metrics, and scalable fabrication makes it a globally impactful contribution to energy storage research.

4. A Charge-Reinforced Ion-Selective Membrane for Long-Lifespan Polysulfide-Based E-Fuel Systems

Polysulfide-based e-fuels hold great promise for large-scale energy storage due to their high solubility (~8.8 mol L^{-1} H_2O) and low chemical cost (~\$0.15 kAh^{-1}). However, their commercialization is severely hindered by challenges such as polysulfide crossover and self-discharge, which lead to rapid capacity fading (typically within 50–60 cycles or 4–25 days without electrolyte refreshment). Despite decades of efforts from academia and industry, effective approaches to extend the lifespan of polysulfide-based e-fuel systems have been elusive. This study made a significant breakthrough with the development of a charge-reinforced ion-selective (CRIS) membrane, addressing these long-standing issues. Below are our key accomplishments:

4.1. Innovation in Ion-Selective Membrane Design:

- The CRIS membrane effectively mitigates polysulfide and polyiodide crossover by leveraging its charge-reinforced ion selectivity, which traps and accumulates negatively charged anions and electrostatically repels active anions in the electrolyte.
- This membrane also restrains swelling, reduces water/OH^- transportation, and ensures the full conversion of electrochemical reactions in each compartment.

4.2. Enhanced Electrochemical Performance:

- The conductive Ketjenblack carbon incorporated into the CRIS membrane facilitates complete electrochemical reactions in each electrode compartment, further improving energy efficiency and system stability.
- This innovation directly addresses the degradation mechanisms that have historically limited the lifespan of polysulfide-based systems.

4.3. Exceptional Longevity and Stability:

- A polysulfide/iodide static cell utilizing the CRIS membrane demonstrated an ultra-low capacity decay rate of 0.005%/day (0.0004%/cycle) over 2.9 months (1,200 cycles) at 100% state-of-charge.

- This represents a dramatic improvement over conventional membranes, extending the lifespan of polysulfide-based systems by orders of magnitude.

4.4. Validation of Prototype Flow System:

- A full-flow prototype system with a 4.0 M KI/2.0 M K_2S_2 electrolyte demonstrated stable cycling at a volumetric capacity of 17.9 Ah L^{-1} (posolyte + negolyte) for over 3.1 months (500 cycles).
- These results highlight the scalability and practicality of the CRIS membrane for real-world applications.

4.5. Impact on Large-Scale Energy Storage:

- By addressing the critical challenges of crossover and self-discharge, the CRIS membrane enables polysulfide-based e-fuels to achieve long lifespans and stable cycling performance, making them a viable candidate for scalable, cost-effective energy storage solutions.
- The technology's potential to reduce system costs and improve reliability aligns with the demands of grid-scale energy storage and renewable energy integration.

This work represents a significant step toward overcoming the technical barriers that have historically hindered polysulfide-based e-fuel systems. The development of the CRIS membrane not only advances the field of e-fuel storage but also provides a pathway for the commercialization of low-cost, high-capacity, and long-lasting energy storage technologies. Its combination of innovative design, exceptional performance metrics, and practical scalability underscores its potential for global impact.

<u>5. A Multilayer Porous Polybenzimidazole Membrane with Ultrahigh Ion Selectivity for Aqueous E-Fuel Chargers</u>

The development of aqueous e-fuel systems is significantly limited by the ion crossover and high cost of commercial Nafion membranes, which impede their scalability and practicality. Polybenzimidazole (PBI)-based membranes, known for their excellent ion selectivity and low cost, have emerged as promising alternatives. However, dense PBI membranes suffer from low proton conductivity due to their inherently narrow and tortuous ion transport channels, even after H_2SO_4 treatment. To address this challenge, we developed a novel multilayer porous PBI membrane using a controlled non-solvent phase separation method. Below are our key accomplishments:

5.1. Innovative Multilayer Structure Design:

- The membrane features a unique sponge-like nanoporous layer/finger-like microporous layer/thin dense layer structure, where:
- The nanoporous layer and thin dense layer effectively block vanadium ion crossover, ensuring excellent ion selectivity.
- The microporous layer provides a "proton transport freeway," reducing area resistance and enhancing proton conductivity.
- This multilayer design overcomes the typical trade-off between ion selectivity and proton conductivity in conventional PBI membranes.

5.2. Ultrahigh Ion Selectivity and Low Area Resistance:

- The multilayer membrane achieves ultrahigh ion selectivity, effectively preventing vanadium ion migration while maintaining low area resistance.
- This performance represents a significant improvement over traditional Nafion and dense PBI membranes, making it a strong candidate for advanced e-fuel systems.

5.3. Facile and Cost-Effective Fabrication Method:

- The non-solvent phase separation method employed for membrane preparation is straightforward, controllable, and cost-effective, requiring relatively low capital investment. - Unlike conventional porous membranes with insufficient ion-blocking capabilities, this method allows precise control over the membrane structure, enhancing both performance and scalability.

5.4. Tunable Thickness for Optimal Performance:

- By adjusting the evaporation time during fabrication, the thickness ratio of the microporous to nanoporous layers can be fine-tuned, enabling an optimal balance between ion selectivity and proton conductivity.
- This tunability ensures the membrane can be tailored for different e-fuel system requirements, enhancing its versatility.

5.5. Advancing Aqueous E-Fuel Technology:

- The combination of low cost, ultrahigh ion selectivity, and excellent proton conductivity makes this multilayer porous PBI membrane a transformative step forward for aqueous e-fuel chargers.
- Its performance advancements directly address the limitations of Nafion membranes, providing a scalable and economically viable alternative for large-scale energy storage systems.

This work represents a breakthrough in membrane design, combining innovative structural engineering with practical fabrication techniques to deliver a high-performance, low-cost solution for aqueous e-fuel systems. The multilayer porous PBI membrane paves the way for next-generation e-fuel chargers by significantly improving ion selectivity and reducing costs, thus enhancing the feasibility of renewable energy storage and utilization.

6. A Novel Electrode with Electrospun Nano- and Micro-Scale Carbon Fibers for Aqueous E-Fuel Chargers

Carbon fibers are the most commonly used electrode materials in e-fuel cells, but their fixed fiber diameter (~10 μm in commercial carbon felt and carbon cloth) creates a trade-off between specific surface area and permeability. To address this limitation, we developed a novel carbon electrode with electrospun nano- and micro-scale fibers, achieving an optimized balance between surface area and permeability. Below are our key accomplishments:

6.1. Innovative Dual-Diameter Fiber Design:

- By combining nano-scale fibers for increased specific surface area and micro-scale fibers for improved permeability, the electrode achieves superior performance compared to conventional single-diameter fibers.
- This dual-diameter design effectively resolves the inherent trade-offs in carbon felt and cloth, ensuring enhanced electrochemical responsiveness and fluid flow efficiency.

6.2. Facile and Tunable Fabrication Process:

- Electrospinning of polyacrylonitrile (PAN) precursor solutions were used to fabricate the carbon fibers, with the fiber diameter controlled by adjusting humidity and collector rotation rates:
- Increased humidity and reduced collector rotation rate led to the formation of large fiber bundles.
- Reduced humidity and increased rotation rates promoted the formation of smaller, single fibers.
- This controllable fabrication process allows precise tuning of fiber morphology to meet specific application requirements.

6.3. Superior Structural Properties:

- The as-prepared dual-diameter carbon electrodes exhibited double the specific surface area of large-fiber electrodes and a 1.4 times higher hydraulic permeability compared to small-fiber electrodes.
- This balance ensures optimal ion transport and solution flow, critical for high-performance aqueous e-fuel chargers.

6.4. Direct Application with No Post-Treatment:

- Unlike many commercial electrodes, the electrospun carbon fibers do not require additional post-treatment and can be directly applied after carbonization, simplifying processing steps and reducing costs.

6.5. Enhanced Vanadium-Based E-Fuel System Performance:

- The vanadium-based e-fuel system equipped with the as-prepared electrodes achieved an 84.78% energy efficiency at a current density of 100 mA cm^{-2}, a significant improvement over conventional electrodes.
- The system also demonstrated stable cycling performance, highlighting the electrode's durability and practical applicability.

6.6. Scalability and Versatility:

- The electrospinning process is cost-effective and scalable, making it suitable for large-scale production of electrodes for various aqueous e-fuel systems.
- The dual-diameter fiber approach can also be tailored to other energy storage systems requiring optimized surface area and permeability.

This research offers a transformative solution for electrode design in aqueous e-fuel chargers. By combining nano- and micro-scale fibers, the novel electrode achieves a superior balance between specific surface area and permeability, enabling enhanced energy efficiency and stable cycling. This breakthrough not only addresses long-standing limitations of commercial carbon materials but also provides a scalable and cost-effective pathway for advancing e-fuel technology.

7. Uniform Distributions of Reactants via Aligned Electrode Design for E-Fuel Chargers and Dischargers

A uniform reactant distribution is critical for improving the performance of flow-field structured e-fuel systems. Enhancing the hydraulic permeability of electrodes in both the through-plane and in-plane directions can significantly reduce concentration overpotential and improve energy efficiency. This work presents a novel approach to electrode design by fabricating uniaxially aligned carbon fiber electrodes, with tailored fiber orientations to optimize reactant flow and battery performance. Below are our key accomplishments and findings:

7.1. Fabrication of Uniaxially Aligned Carbon Fiber Electrodes -
Electrospinning Process:

- Electrospun carbon fiber electrodes with diameters ranging from 7 to 12 μm (average ~10 μm) were fabricated, achieving a uniaxial alignment.
- The aligned structure enhances hydraulic permeability compared to conventional randomly oriented electrospun fibers, facilitating reactant distribution.

7.2. Enhanced Battery Performance -
Energy Efficiency Improvement:

- The battery assembled with aligned fiber electrodes exhibited an energy efficiency of 84.4% at 100 mA cm^{-2}, representing a 13.2% improvement compared to conventional electrospun fiber electrodes.
- This enhancement is attributed to the higher permeability of the aligned structure, which promotes a more uniform reactant distribution and reduces concentration overpotential.

7.3. Optimization of In-Plane Permeability by Adjusting Fiber Orientation -
Tailored Fiber Orientation:
- By adjusting the orientation of aligned fibers relative to the flow channels, the in-plane permeability was optimized:
- Perpendicular Orientation: When the aligned fibers were oriented perpendicular to the flow channel direction, the battery achieved the largest discharge capacity and the highest limiting current density (~900 mA cm^{-2}).
- This orientation maximized reactant distribution and current uniformity, directly improving battery performance.

- Impact on Reactant Distribution:
- The perpendicular alignment facilitates uniform reactant flow across the electrode surface, reducing concentration gradients and enabling efficient electrochemical reactions.

7.4. Validation via Three-Dimensional Modeling -
3D Model Insights:
- A three-dimensional model corroborated the experimental findings, showing that the perpendicular alignment of fibers relative to flow channels results in the most uniform in-plane reactant and current distribution.
- This uniformity minimizes concentration overpotential and enhances the overall performance of the e-fuel system.

7.5. Key Contributions to E-Fuel System Design
(1) Improved Reactant Distribution:
- The aligned fiber structure promotes uniform reactant flow, reducing concentration overpotential and enabling higher energy efficiency.

(2) Enhanced Performance Metrics:
- The tailored electrode design increased battery energy efficiency by 13.2% and achieved a high limiting current density of ~900 mA cm^{-2}, demonstrating significant performance gains.

(3) Scalable and Practical Fabrication:
- The electrospinning process for uniaxially aligned fibers is scalable and cost-effective, making it suitable for large-scale e-fuel systems.

(4) Customizable Design for Flow-Field Systems:
- The ability to optimize fiber orientation relative to flow channels offers a versatile approach for improving the performance of various flow-field structured systems.

Impact and Future Directions
This study has provided a transformative approach to electrode design for e-fuel chargers and dischargers. By leveraging uniaxially aligned carbon fiber electrodes, the work has addressed one of the fundamental challenges in e-fuel systems—uniform reactant distribution. The results demonstrate the potential for significantly enhanced energy efficiency and system performance, paving the way for further optimization and application in advanced energy storage

technologies. Future work can explore the integration of these electrodes into larger-scale systems and investigate their long-term stability under real-world operating conditions.

8. Mathematical Modeling of E-Fuel Cells Incorporating Shunt Current and Thermal Effects

The development of advanced mathematical models is critical for understanding and optimizing e-fuel systems, including their chargers and power packs. This work integrates coupled transport and reaction processes with detailed thermal and shunt current modeling to improve the design and performance of next-generation high-power-density e-fuel systems. Below is a summary of our major advancements and findings:

8.1. Coupled Transport and Reaction Processes -

Comprehensive Numerical Model:

- The model simulates species transport, charge transport, fluid flow, and electrochemical reactions in both the e-fuel charger and power pack.
- This coupled approach ensures accurate representation of the complex interactions within e-fuel cells, enabling better predictions of system behavior.

- Electrode Optimization via Numerical Design:
- New electrode structures for the e-fuel charger and power pack were numerically designed to enhance performance.
- The optimization focused on improving reactivity, surface area, and reactant transport efficiency.

8.2. Shunt Current Modeling -

Equivalent Circuit Model:

- Shunt current loss was modeled using an equivalent circuit approach, where:
- Flow channels act as resistors,
- Manifolds between cells in series act as additional resistors, - The discharge voltage acts as a voltage source.
- This approach accommodates e-fuels with varying physical and chemical properties by assigning corresponding resistances.

- Key Insights:
- The model quantifies shunt current losses and enables design improvements to minimize these losses, enhancing overall system efficiency.

8.3. Thermal Modeling -

Improved Thermal Model:

- The thermal model incorporates a heat transfer network for all major components, with internal resistance dynamically varying with temperature and state of charge.
- Concentration overpotential differences between charge and discharge processes were also included to improve accuracy.

- Key Features:
- The model predicts electrolyte temperature variations under different operating modes. - Heat generation rates from electrochemical reactions, resistive losses, and side reactions are analyzed, providing insights for heat source control.

- Impact:
- This thermal model supports the development of thermal management strategies, ensuring stable operation and longer system lifespans.

9. 3D Mathematical Modeling of E-Fuel Cells

To further improve electrode performance, a three-dimensional numerical model was developed, incorporating porosity-graded electrode designs. This model focuses on anisotropic transport properties and their influence on large- and small-scale e-fuel systems.

9.1. Graded Electrode Design -
Anisotropic Permeability:
- Unlike previous models assuming isotropy, this work considers anisotropic permeability, with permeability coefficients varying spatially within the electrode.
- This approach accounts for realistic flow patterns and reactant transport in the electrode.

- Balancing Surface Activity and Structure:
- The optimized electrodes balance surface activity (reactivity) with macroscopic and microscopic structural properties.
- By adjusting porosity and fiber diameter, a larger specific surface area and better mass transfer are achieved.

9.2. Large-Scale vs. Small-Scale Systems -
Flow Pattern Optimization:
- For large-scale systems, the flow per unit area is lower, making concentration polarization a significant source of loss.
- The optimization focuses on increasing porosity to ensure uniform reactant distribution across the entire electrode.

- Permeability Direction Control:
- Permeability direction can be optimized to improve mass transfer, but care must be taken to avoid reducing the specific surface area, which would increase activation losses.

- Fiber Surface Modification:
- To compensate for reduced specific surface area due to increased porosity, fiber surfaces are modified to enhance reactivity and maintain high performance.

9.3. Toolkit for Large-Scale Optimization
- The three-dimensional numerical toolkit developed in this study can be applied to optimize:
  - Flow Patterns: Designing flow fields to minimize concentration polarization and improve reactant distribution.
- Electrode Structures: Optimizing porosity, fiber diameter, and permeability direction to enhance mass transfer and reactivity.
- Thermal Management: Integrating the thermal model to control heat generation and maintain stable operation.

Key Contributions and Impacts
1. Comprehensive Modeling Framework:
- The integration of shunt current, thermal effects, and anisotropic transport properties provides a holistic approach to optimizing e-fuel systems.

2. Enhanced Electrode Performance:

- The porosity-graded electrode design ensures uniform reactant distribution, reduced concentration polarization, and improved mass transfer efficiency.

3. Scalability:
- The models address the unique challenges of large-scale e-fuel systems, providing insights into flow pattern optimization and electrode design for high-power applications.

4. Thermal Management:
- The improved thermal model supports effective heat source control, enabling stable and efficient operation under varying conditions.

5. Design Optimization Toolkit:
- The developed 3D numerical toolkit enables targeted optimization of flow fields, electrodes, and thermal management strategies, paving the way for the next generation of high-performance e-fuel systems.

This work has established a robust foundation for optimizing e-fuel systems, providing tools and insights to advance their performance, scalability, and commercial viability.

10. Novel Machine Learning-aided Data Driven Approaches to Design Electrodes and Flow Fields

10.1. Optimization of E-Fuel Electrode Structures

Accomplishment: The team generated a dataset of 2,275 fibrous structures using a combination of stochastic reconstruction, morphological algorithms, and lattice Boltzmann modeling. By applying machine learning regression models and genetic algorithms, 700 optimal solutions were identified, achieving an up to 80% larger specific surface area and a 50% higher hydraulic permeability compared to commercial graphite felt electrodes.
International Excellence: This work provides a data-driven design framework for high-performance electrodes, advancing the field of energy storage. The results have been presented at international conferences and published in high-impact journals, reflecting their academic and practical significance.

10.2. Development of a Generative Adversarial Network (GAN) for Microstructure Reconstruction

Accomplishment: A GAN-based technique was developed to reconstruct the three-dimensional microstructure of e-fuel electrodes. The method achieved high-quality image synthesis, validated through statistical comparisons (porosity, specific surface area, tortuosity, and two-point correlation function) and t-distributed stochastic neighbor embedding (t-SNE) analysis. The GAN demonstrated the capability to generate larger images with high computational efficiency and scalability, with computation time scaling linearly with image size.
International Excellence: This work represents a cutting-edge application of machine learning in energy materials design. The use of GANs for microstructure reconstruction has been recognized as a pioneering effort and has potential applications beyond e-fuel systems, contributing to broader advancements in materials science.

10.3. Design and Optimization of Flow Fields for E-Fuel Systems

Accomplishment: A library of 11,564 one-channel flow fields was created using a custom path generation algorithm encoded as binary images. Collaborative screening identified eight novel designs that, when experimentally validated, showed a 22% higher limiting current density and an 11% improved energy efficiency compared to conventional serpentine flow fields. Quantitative design rules were established, revealing optimal channel length and torque integral parameters. The method was extended to two-channel flow fields, generating 11,600 designs and identifying candidates with superior electrochemical performance to conventional interdigitated flow fields.

International Excellence: This systematic approach to flow field design, grounded in computational modeling and experimental validation, has set a new benchmark in the field. The results have been highlighted in peer-reviewed journals and are being explored for industrial applications.

10.4. Integration of Machine Learning and Experimental Validation

Accomplishment: The integration of machine learning tools, such as regression models, genetic algorithms, and GANs, with experimental validation has significantly accelerated the discovery of high-performance materials and components for e-fuel systems. This multidisciplinary approach enabled the identification of optimal electrode structures and flow field designs with unprecedented efficiency.

International Excellence: The innovative combination of computational modeling, machine learning, and experimental validation has been recognized as an example of cutting-edge research methodology. The techniques developed are applicable across a wide range of energy storage technologies, further enhancing their impact.

10.5. Creation of a Comprehensive Design Framework for E-Fuel Systems

Accomplishment: This work has delivered a comprehensive, data-driven framework for designing key components of e-fuel systems, including electrodes and flow fields. This framework combines computational modeling, machine learning, and experimental validation to optimize performance metrics such as specific surface area, hydraulic permeability, and electrochemical efficiency.

International Excellence: The framework has been widely acknowledged for its potential to revolutionize the design of energy storage systems. Publications in high-impact journals and presentations at international conferences have demonstrated the global relevance and applicability of this work.

Conclusion

These accomplishments showcase the team’s ability to combine advanced computational methods, machine learning, and experimental validation to address critical challenges in e-fuel systems. The innovative methods and high-impact outcomes have achieved international recognition, setting a strong foundation for further advancements in energy storage technologies.

11. Scaling and Integration of E-Fuel Energy Storage Systems for High-Efficiency Applications

The multi-scale electrodes, high-selectivity membranes, and optimized flow field designs developed in this project were integrated into scaled-up e-fuel systems whose performance in real-world applications were validated. Below is a summary of our major accomplishments and research highlights:

11.1. Development and Validation of a 1 kW E-Fuel Charger and Power Pack -

Design and Configuration:

- The 1 kW e-fuel charger and 1 kW e-fuel power pack consisted of 10 single cells, each with a reaction area of 400 cm^2.
- A face seal structure using fluororubber (FPM) and polytetrafluoroethylene (PTFE) sheets was employed to ensure effective sealing.

- Performance Metrics:
- The e-fuel charger showed a charge efficiency of 94.7% at a charging current density of 50 mA cm^{-2}.

- The e-fuel power pack demonstrated a discharge efficiency of 95.0% at an operating current density of 200 mA cm^{-2}.
- The system achieved an overall round-trip efficiency of 90.0%, validating the high efficiency of this e-fuel energy storage system.

11.2. Scaling Up to a 2 kW E-Fuel Power Pack -
Design and Configuration:
- The 2 kW e-fuel power pack was built with 8 single cells, each featuring a larger reaction area of 1,000 cm^2.

- Performance Metrics:
- At a rate current density of 200 mA cm^{-2}, the power pack achieved a discharge power of 2.5 kW at 250 mA cm^{-2}.
- The discharge efficiency remained as high as 96%, even at a current density of 200 mA cm^{-2}, demonstrating excellent energy conversion efficiency.

- Integrated System:
- A 1 kW e-fuel charger and a 2 kW e-fuel power pack were integrated with a shared piping system.
- The integrated system achieved a round-trip efficiency of 92.3%, confirming the high efficiency and scalability of the e-fuel energy storage system.

11.3. Assembly and Validation of a 10 kW E-Fuel Charger and Power Pack -
10 kW E-Fuel Charger:
- The charger used a flow-through structure with 38 single cells (19+19), each with an active area of 600 cm^2.

- Performance:
- Charge power of 5.6 kW at 50 mA cm^{-2}, increasing to 10 kW at 100 mA cm^{-2}.

- 10 kW E-Fuel Power Pack:
- The power pack employed an advanced flow-by structure for superior performance under higher current densities.
- Performance:
- Discharge power of 10 kW at 160 mA cm^{-2}, increasing to 12.5 kW at 200 mA cm^{-2}.

11.4. Integration of a 10 kW Solar-Powered E-Fuel Energy Storage System -
System Components:
- The 10 kW e-fuel charger, 10 kW e-fuel power pack, two 300 L electrolyte tanks, pumps (0.75 kW), a 2 P cooler, a piping system, and a battery management system were assembled on a test platform.
- The system was powered by a 10 kW solar energy system, consisting of 33 solar panels (330 W each) installed on the rooftop of a building at HKUST.

- Performance Metrics:
- The system powered an AC load of 6 kW and achieved a round-trip efficiency of 92.3%, demonstrating its high efficiency and potential for renewable energy applications.

Key Contributions and Impact (1)
Scalable and Modular Design:
- The integration of the 1 kW, 2 kW, and 10 kW systems demonstrated the scalability of e-fuel energy storage for different power demands, from small-scale applications to grid-scale systems.

(2) High Efficiency and Stability:
- The systems consistently achieved high round-trip efficiencies (90.0–92.3%) and stable cycling performance, validating the e-fuel platform's potential for long-term deployment.

(3) Renewable Energy Integration:
- The successful coupling of the 10 kW e-fuel system with solar panels highlights its feasibility for renewable energy storage, providing a sustainable solution for low-carbon energy systems.

(4) Advanced Material Utilization:
- The use of PBI membranes, graphite plates, and optimized flow field designs enhanced system performance, enabling high charge/discharge efficiencies and energy densities.

(5) Pathway to Commercialization:
- The development of a 10 kW solar-integrated e-fuel system marks a significant milestone toward commercial-scale implementation, showcasing its capability to store renewable energy efficiently and reliably.

This work demonstrates the practical potential of e-fuel energy storage systems for high-efficiency, scalable, and renewable energy applications, paving the way for future advancements in sustainable energy storage solutions.

6.2 What was the added value of the TRS funding, rather than standard project grant funding?
(For example, could this work have been achieved with other funding scheme, such as the General Research Fund or Collaborative Research Fund? If not, why?)

The Theme-based Research Scheme (TRS) funding provided essential support for this work which could not have been achieved through standard funding schemes like the General Research Fund (GRF) or Collaborative Research Fund (CRF). Its unique value is outlined below:

Enabling Large-Scale Multidisciplinary Collaboration
TRS funding facilitated collaboration across multiple disciplines, institutions, and research teams to tackle the complex challenges of this project. Standard schemes such as the GRF or CRF lack the scope and budget to support projects of this scale.

Support for Ambitious Research Objectives
The project's comprehensive goals, including advancements in electrocatalysis, materials development, thermal management, and system scaling, required significant resources and coordination. Such multifaceted objectives could not be achieved under the narrower scope of the GRF and CRF.

Advancement of High-Impact Technologies
TRS enabled the development of over eight novel compounds, advanced membranes, and multiscale electrodes, as well as the filing of two US patents and seven Chinese patents. These outcomes demanded substantial resources and collaboration beyond the scope of the GRF or CRF.

Facilitating Industrial Collaboration and Technology Transfer
TRS funding supported partnerships with institutions like Argonne National Laboratory and promoted industry engagement to advance commercialization. Standard schemes such as GRF focus on academic research and provide limited support for industrial applications.

Alignment with Hong Kong's Strategic Goals
TRS funding directly contributes to Hong Kong's sustainability objectives by supporting renewable energy technologies with significant long-term economic and environmental impacts.

In general, TRS funding was critical to the success of this project, enabling large-scale collaborations, ambitious research, and transformative technological advancements. Standard grants like GRF or CRF cannot provide the necessary resources to achieve the project's objectives and societal benefits.

6.3 If the project has not met its original objectives, why?

N/A

6.4 (a) Please provide details of each peer-reviewed journal publication arising <u>directly</u> from this project by completing the table at **<u>Annex</u>** *(one for each publication)*.

Since the start of the project, we have published a total of 142 journal papers, which are listed in the Appendix.

(b) Please provide details of recognised international conference(s) in which paper(s) related to this project was/were delivered by completing the following table:
<u>(Please attach a copy of each conference abstract)</u>

Since the start of the project, we have published a total of 24 conference papers, which are listed in the Appendix.

(c) RGC funding should have been acknowledged in all publication(s)/conference papers listed in (a) and (b) above. If no acknowledgement has been made in any of the publications/ papers, please indicate and provide explanations.

N/A

6.5 To what extent this project has strengthened inter-institutional collaborations and other partnerships?

This project has significantly enhanced inter-institutional collaborations through joint research, co-supervision of students, and collaborative funding applications. Key highlights include:

1. Collaborative Research:
- Prof. Y.C. Lu and Prof. T.S. Zhao combined experimental approaches and DFT calculations to study sulfur utilization.
- Prof. Q. Chen partnered with Profs. G.C. Jia, T.S. Zhao, and J.K. Kim for the design of organic e-fuel systems and e-fuels with a high energy density and for the optimization of electrodes.
- Profs. P. Gao, M.H. Shao, and K.Y. Chan jointly developed high-performance membranes and multi-scaled electrodes.
- Prof. L. An worked with Prof. T.S. Zhao to develop single e-fuel air systems with a high energy density.

2. Co-Supervision of Students:
- Team members co-supervised PhD candidates Mr. Yang Li, Mr. Bin Liu, Mr. Chun Wai Tang, Ms. Jing Sun, and other students, fostering academic ties and training future researchers.

3. Joint Publications and Funding:
- Collaborations between Profs. G.C. Jia and T.S. Zhao led to multiple publications on redox-active molecules.

- The team successfully applied for two new RGC CRF projects, with two other proposals submitted and pending funding decisions.

4. Interdisciplinary Expertise:

- The partnerships integrated expertise in electrocatalysis, numerical modeling, and material development, expediting advancements in e-fuel systems.

In summary, the project has strengthened partnerships by fostering collaboration, expanding networks, and advancing e-fuel technologies through shared expertise and resources.

6.6 Research students trained (registration/awards):

A total of 27 research students have been trained and supported by this project. The list of students is provided in the Appendix.

6.7 Specific products (e.g. software or netware, instruments or equipment developed):

We developed more than eight types of redox-active compounds or composite nanomaterials used as active species in e-fuels. We also developed low-cost polyethylene and PBI composite membranes with high ionic conductivity. More than five types of modification methods were developed for the electrodes, which are suitable for large-scale production.
We have also designed and assembled a piece of equipment that can conduct in situ Raman tests inside the cells. This equipment has various uses in in situ investigations of electrochemical processes.

6.8 Other education activities and/or training programmes developed:
The research team has co-organized several seminars and workshops to provide tutorial lectures particularly for junior researchers, including a joint workshop with GP Batteries, an industry workshop on new developments in energy storage, and a lecture on fast-charging batteries vs. high-energy-density batteries for electric vehicles. The research team members have also supervised several undergraduate final-year projects in the area of energy storage.

6.9 Please highlight any deliverables indicated in the project implementation timetable endorsed by the RGC which have not been covered or achieved as per sections 6.1 to 6.8 above, and explain/ elaborate. N/A.

Project Management

6.10 Please elaborate how the PC has played his/her role in coordinating and managing the project. The Project Coordinators (PCs), Prof. T.S. Zhao and Prof. Minhua Shao, provided strong leadership to ensure the success of the TRS project.

1. Leadership and Coordination

Prof. T.S. Zhao: As the first PC, Prof. Zhao facilitated collaboration among team members and external partners, monitored research directions, and ensured alignment across all tasks. He co-hosted research activities and fostered partnerships, including those with external institutions such as Argonne National Laboratory.

Prof. Minhua Shao: In January 2022, Prof. Shao took over as PC, focusing on strategic oversight and grant management. He leveraged his expertise in Li-ion batteries and fuel cells to guide progress in Tasks 1 and 6, while promoting interdisciplinary collaboration within the team. **2. Budget and Resource Management**

Both PCs ensured efficient resource allocation and budget management as approved by the Executive Committee.

3. Supervision and Monitoring

Both PCs actively supervised students and researchers, monitored research progress, and ensured timely completion of deliverables. After Prof. Shao took over as PC, Prof. Zhao continued to contribute as a Co-PI, participating in meetings and overseeing Tasks 1, 4, 5, and 6, while Prof. Shao dedicated additional time to steering the project.

4. Public Outreach and Industry Collaboration

The PCs promoted project outcomes to the public and media. While Prof. Zhao focused on promoting e-fuel technologies in mainland China, Prof. Shao made efforts to strengthen industry engagement to facilitate technology transfer and commercialization.

5. Ensuring Continuity

Prof. Zhao and Prof. Shao collaborated to ensure a seamless leadership transition and that research productivity was maintained and activities were aligned with project objectives.

Both PCs played critical roles in managing collaborations, resources, and research progress, ensuring the project was on track to achieve impactful outcomes in energy storage technology.

7. Awards and Recognition

7.1 Have any research grants been awarded that are directly attributable to the results obtained from this project?

During the reporting period, the research team applied for a total of four CRF projects that are related to this project, two of which have been funded. Please refer to the Appendix.

7.2 Have any project team members participated as invited speakers in or organisers of international conferences as a result of this project?

Prof. T.S. Zhao was invited to two international conferences as keynote speakers to give talks about e-fuel energy storage systems during the reporting period, including: (1) The 3rd International Symposium on Insulation and Discharge; and (2) The 2nd International Symposium on Measurement Technology in Thermal Science and Engineering, MTTSE-2019.

Prof. Y.C. Lu was also invited to two international conferences to give speeches on the research progress of this project, including: (1) The World Congress on Green Intelligent Manufacturing Technology; and (2) Hong Kong Symposium of Batteries.

7.3 Have any project team members taken leadership positions in editorial boards, scientific and professional organisations?

(1) Prof. Y.C. Lu has been appointed as a member of the Editorial Board for Materials since 01/01/2019.

(2) Prof. T.S. Zhao has been appointed as the Editor-in-Chief of the International Journal of Heat and Mass Transfer (Elsevier) since 01/01/2019.

(3) Prof. M.H. Shao has been:

Editorial Board Member, Electrocatalysis, 2019-

Treasurer, Energy Technology Division, The Electrochemical Society, 2019-

Vice Chair, Division 5 (Electrochemical Process Engineering and Technology) of the International Society of Electrochemistry, 2019-

Chair, Internal Affairs Committee, The Hong Kong Young Academy of Sciences, 2019.

7.4 Any documentary proof of the application of technologies arising directly from this project?

N.A.

7.5 Other awards and recognitions as a result of this project (please specify):

1) Prof. T.S. Zhao, PI of this project, was elected as an Academician of the Chinese Academy of Sciences (CAS). Prof. T.S. Zhao was also named a Highly Cited Researcher in 2020 by Web of Science.
2) Prof. Y.C. Lu (Co-leader of Task 1) won the National Science Fund for Distinguished Young Scholars.
3) Prof J.K. Kim, Professor Emeritus of Mechanical and Aerospace Engineering, was named a Highly Cited Researcher in 2020 by Web of Science.
4) Prof. Q. Chen received the 2020 Excellent Young Scientist (EYS) Scheme award from the National Natural Science Foundation of China (NSFC), a highly prestigious honor in China.

8. Impacts

8.1 What are the current and expected impacts of the project on the long-term development of Hong Kong (social or economic development, e.g. patent, technology transfer, collaboration with external organisations, etc.)?

This project has significant social and economic impacts on Hong Kong, both now and in the future. Key impacts include:

Environmental Sustainability:
The e-fuel energy storage system is clean, renewable, and environmentally friendly, with no harmful precious metals and fully recyclable e-fuel, addressing the limitations of non-recyclable lithium-ion and lead-acid batteries.
It aligns with Hong Kong's aggressive carbon reduction targets by offering alternative renewable energy solutions, reducing reliance on fossil fuels, and lowering the carbon footprint.
Technological Advancements:
Development of high-performance components, including 8+ new compounds, PE- and PBI-based membranes, and multiscale electrodes, which have applications beyond e-fuel systems in flow batteries and fuel cells. Filing of 2 US patents and 7 Chinese patents demonstrates innovation with potential for global impact.
Economic Benefits:
The theoretical 20-year lifespan and low-cost, high-performance materials reduce costs for renewable energy systems, offering significant economic benefits.
The project supports the industrialization of e-fuel systems, positioning Hong Kong as a leader in energy storage technology.
Collaborations and Recognition:
Collaborations with external institutions, such as Argonne National Laboratory, have yielded high-impact publications (e.g., Nature Nanotechnology).
Active engagement with industries promotes future technology transfer and commercialization opportunities, driving economic growth.
Broad Application Prospects:
The kilowatt-scale e-fuel system being tested has applications in stationary energy storage and beyond, paving the way for widespread adoption in renewable energy systems.
In summary, the project contributes to Hong Kong's sustainability goals, advances energy storage technology, fosters industrialization, and brings economic benefits, positioning the city as a hub for clean energy innovation.

8.2 Others (please specify):

During the reporting period, the PC and team members actively promoted the project outcomes to foster collaborations with external institutions and industries. These efforts included:

Proactive Dissemination:

Project results were shared at various events and platforms to highlight the advancements in e-fuel energy storage systems and their potential applications.

Engagement with Institutions and Industries:

Promotions aimed at establishing partnerships have created opportunities for future collaborations with academic institutions and industrial stakeholders, driving the potential for technology transfer and commercialization. **Media Coverage:**

The project gained visibility through several news reports, showcasing its significance and impact. Details of the reports are listed in the Appendix.

These activities have strengthened the project's outreach, laying the groundwork for expanding collaborations and accelerating the adoption of e-fuel technologies.

9. Sustainability of the Project

9.1 Whether there are new ideas evolved directly from this project?

Several innovative ideas have emerged directly from this project. The team has successfully developed more than eight novel compounds and materials, including advanced composite membranes and multiscale electrodes, which have applications beyond e-fuel systems, such as in flow batteries and fuel cells. Additionally, the concept of recyclable and environmentally friendly e-fuels has inspired further exploration into alternative energy storage solutions for both stationary and portable applications.

9.2 Whether there are new projects evolved directly from this project?

This project has directly led to the initiation of several new research endeavors. Two Research Grants Council (RGC) Collaborative Research Fund projects have been secured, and additional proposals, including an RGC Theme-based Research Scheme project and a National Key R&D Program, are currently under review. These new projects build upon the foundational research of e-fuels, focusing on scaling up systems, optimizing components, and exploring new applications for energy storage systems.

9.3 Whether there are new collaborations developed directly from this project?

The project has facilitated the development of new collaborations with both academic institutions and industrial partners. A key collaboration with Argonne National Laboratory resulted in a high-impact publication in Nature Nanotechnology. Furthermore, the team has actively engaged with industrial stakeholders to promote the commercialization of e-fuel technologies, laying a strong foundation for future technology transfer and industrial applications.

9.4 Please give details on how much money and from which sources has been obtained/requested for the specific purpose of continuing the work started under this project.

Funding has been secured for two new RGC Collaborative Research Fund (CRF) projects to continue the work initiated under this project. In addition, two new proposals have been submitted to the RGC Theme-based Research Scheme and the National Key R&D Program. Both proposals aim to further advance the development, optimization, and industrialization of e-fuel systems.
These efforts to obtain funding demonstrate the sustainability and long-term potential of the research initiated through this project.

10. Statistics on Research Outputs

(Please ensure the statistics in this section are consistent with the information presented in other sections of this report.)

	Peer-reviewed journal publications	Conference papers	Scholarly, books, monographs and chapters	Patents awarded	Other research outputs (please specify)	
					Type	No.
No. of outputs arising directly from this research project	142	24	2	20	Awards	4

12. The Layman's Summary

(describe in layman's language the abstracts and research impact of the project.)

Energy storage is a critical technology for renewable energy systems, enabling us to store electricity generated from sources like solar and wind, so it can be used when needed. Our research project has achieved several groundbreaking advancements in liquid energy storage technologies, potentially revolutionizing the way we store and use renewable energy.

Innovative E-Fuels for Energy Storage
The team has developed two new types of liquid fuels (e-fuels) made from advanced materials like boron, silicon, and polychalcogenides. Our boron-based e-fuels are chemically stable and efficient, offering a reliable way to store energy for next-generation batteries. Our sulfur and selenium e-fuels simplify energy storage by eliminating the need for extra chemicals, making this "self-mediating" system cost-effective and scalable. In addition, our silicon-based nanofluids are designed for high energy density and long-term stability by overcoming common issues like material degradation.

Breakthroughs in Membrane Technology
Membranes are critical components in e-fuel systems, as they control the flow of ions (i.e. charged particles) while preventing unwanted material from crossing over. The team has designed new membranes that are cheaper, more efficient, and longer lasting. Our charge-reinforced membranes dramatically reduce energy loss and extend the lifespan of energy systems. Our porous polybenzimidazole (PBI) membranes represent a low-cost, highly efficient alternative to expensive commercial membranes. They offer enhanced ion selectivity and durability.

Improved Electrodes for Energy Storage
Electrodes store and release energy in e-fuel systems. The team has developed advanced carbon fiber electrodes with innovative designs to enhance performance. In one design, combining small-diameter fibers with large-diameter fibers increases the efficiency of energy storage systems while ensuring

durability. In another design, aligning carbon fibers improves the flow of reactants, resulting in more uniform energy storage and higher efficiency.

Mathematical Modeling and Machine Learning

To improve the design of e-fuel systems, the team used advanced computer simulations and machine learning to predict how changes in materials and system designs would affect performance. Detailed simulations using 3D models were conducted to optimize the flow of energy within the system, improving energy efficiency and reducing losses. Machine learning was performed to design better electrodes and flow fields, achieving significant performance improvements.

Scaling up the Technology

The team has successfully built and tested larger e-fuel systems to demonstrate their real-world potential. Our 10 kW system prototypes showed high efficiency, with up to 92% of the energy stored and retrieved effectively. The technology has been designed with scalability in mind, making it cost-effective and practical for larger applications like grid-scale energy storage.

Why This Matters

These accomplishments represent a significant step toward making energy storage systems more efficient, affordable, and scalable. By improving materials, designs, and manufacturing processes, these innovations could lead to cheaper energy storage, making renewable energy more competitive with fossil fuels. They could also result in longer-lasting systems, reducing maintenance and replacement costs. Moreover, these innovations could enable grid-scale applications, allowing for the storage of massive amounts of energy for use in homes, businesses, and industries.

The Future of E-Fuels

The project's advancements pave the way for a sustainable energy future. With further development and commercialization, these technologies could play a key role in transitioning to a world powered by renewable energy.