



## Development of New Synthetic Pathways for Renewable Energy Storage

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### ABSTRACT

Due to the intermittent nature of renewable energy sources (solar, wind), there is a need to develop efficient, scalable, and sustainable energy storage systems. Existing energy storage technologies face fundamental challenges, and this study aimed to tackle those challenges by exploring new synthetic routes for novel materials. It focused on enhancing the performance, scalability, and environmental sustainability of energy storage technologies, including lithium-ion batteries, supercapacitors, and hydrogen storage systems. Designing metal-organic frameworks (MOFs), perovskites and polymer electrolytes via green chemistry principles to minimize the environmental impact of produced materials. The cyclic voltammetric, electrochemical impedance spectroscopic and long-term cycle stability measurements of electrochemical performance were conducted. Density Functional Theory (DFT) simulations for computational modelling were used to predict material properties and optimize reaction pathways. In these results, MOF based Lithium-ion batteries achieved the best energy density (310 Wh/kg); polymer based supercapacitors exhibited high power density (2000 W/kg) and cycling stability (94% retention after 1000 cycles). Recently stability of perovskite-based hydrogen storage systems was improved to 88% of the capacity after 1000 cycles. The results confirmed that using high-performance materials from 21st century fibres with sustainable synthesis approaches solved key performance and sustainability challenges. It lays a foundation towards stackable and sustainable energy storage systems, which can be used in technological energy grids, electric vehicles, and portable devices.

### INTRODUCTION

One key approach in global efforts to address climate change and reduce reliance on fossil fuels is the transition toward renewable energy. Renewable energy resources such as solar and wind are intermittent; thus, there is a need to develop energy storage technologies that are cost-efficient, scalable, and sustainable (Nagarajan et al., 2021). Among those novel synthetic methods for energy storage could become a hope for solving these problems through increasing energy storage efficiency, reducing environmental

impact, and promoting compatibility with renewable energy grids (Dong et al., 2017). This work focuses on developing new synthetic methods that underpin advanced energy storage technologies like batteries, hydrogen storage, and supercapacitors, which are key to achieving sustainable energy systems (Niu et al., 2018).

A large number of recent literature examines energy storage technologies such as lithium-ion batteries, hydrogen fuel cells, and electrochemical capacitors and suggests these technologies could disrupt energy



systems (Liu et al., 2016). Synthetic chemistry explorations have enabled the preparation of novel microstructures of electrodes with higher rate tolerating electrocatalytic processes and more cost-effective retention methods (Ye et al., 2017). Despite these advances, important gaps exist between sustainable methodologies that incorporate scalability and resource availability (Yabuuchi, 2019). Although metal-organic frameworks and perovskites have had great success in laboratory settings, their synthesis and material stability control must still be ameliorated for scaling up (Mo et al., 2017). Thus, these constraints emphasize the importance of continuous efforts on innovative, effective, and environmentally friendly synthetic strategies (Sun et al., 2016).

Thus, this work seeks to fill these gaps through novel syntheses to mitigate challenges associated with renewable energy storage systems' scalability, sustainability, and efficiency production (Liu et al., 2016). Hence, this research work aims for sustainable development of energy storage technologies based on green chemistry using novel and optimized materials and reaction pathways (Shanbhag et al., 2017). So, the aim is to develop processes that optimize energy density and performance while lowering storage systems' environmental footprint (Cheng et al., 2017). The overall goal of this project is to guide the mission to develop a sustainable and large-scale renewable energy infrastructure (Zhu et al., 2020).

## METHODOLOGY

### Research Design

This study utilized a comprehensive experimental and computational methodology to create innovative synthetic routes for renewable energy storage. The process comprises three phases: material synthesis, pathway optimization, and performance evaluation. This study incorporates green chemistry principles, sophisticated synthesis methods, and computational modeling to guarantee environmental sustainability, scalability, and efficiency.

### Material Synthesis

The initial phase includes synthesizing candidate materials, emphasizing unique molecules such as metal-organic frameworks (MOFs), perovskites, and novel polymeric substances. These materials are selected for their capacity to augment energy density, optimize charge-discharge efficiency, and facilitate scalability. The synthesis process involves various techniques summarized in Table 1:

**Table 1**

*Material Synthesis Techniques and Their Objectives*

Technique	Material Targeted	Objective	Key Benefits
Sol-gel synthesis	Nanostructured materials	Enhance surface area and conductivity	Scalable and cost-effective

Hydrothermal/Solvothermal	MOFs, Perovskites	Achieve high crystallinity and purity	Controlled size and morphology
Polymerization processes	Advanced polymer electrolytes	Develop high-performance ion-conducting electrolytes	Lightweight and flexible
Use of green solvents	All materials	Minimize environmental impact	Reduced hazardous waste

### Pathway Optimization

Synthesized materials are integrated into energy storage systems such as lithium-ion batteries, supercapacitors, and hydrogen storage devices. Optimization focuses on electrochemical, catalytic, and structural performance, as summarized in Table 2:

**Table 2**

*Pathway Optimization Methods*

Aspect	Method	Purpose
Electrochemical reactions	Cyclic Voltammetry (CV), EIS, GCD	Evaluate redox kinetics, ion transport, and energy efficiency
Catalytic processes	Catalysis testing for hydrogen storage	Improve hydrogen release and uptake
Thermal stability	Thermogravimetric Analysis (TGA)	Assess material stability under various conditions
Structural stability	X-ray Diffraction (XRD)	Verify crystallinity and phase purity

### Computational Modeling

Computational tools are used to predict material properties and optimize reaction mechanisms. Table 3 highlights the computational methods employed:

**Table 3**

*Computational Modeling Techniques*

Tool/Method	Objective	Expected Outcome
Density Functional Theory (DFT)	Simulate band structures, ionic conductivity	Identify high-performance materials
Reaction Pathway Simulations	Predict reaction intermediates and transition states	Optimize catalytic performance
Molecular Dynamics (MD)	Study structural stability under operational conditions	Enhance robustness of materials

### Performance Evaluation

The optimized energy storage systems are tested for performance based on key metrics, as detailed in Table 4:

**Table 4**

*Performance Metrics for Energy Storage Systems*

Metric	Testing Method	Significance
Energy density	Galvanostatic charge-discharge tests	Evaluate practical storage capacity
Power density	Electrochemical impedance spectroscopy (EIS)	Measure rapid energy delivery potential
Cycling stability	Long-term charge-discharge cycles	Assess durability over time
Environmental impact	Life Cycle Analysis (LCA)	Evaluate ecological footprint
Scalability	Industrial-scale simulation	Test feasibility for large-scale production

## Data Analysis

Experimental and computational data are analyzed using statistical tools to ensure reproducibility and reliability. Comparative analyses are performed to benchmark the results against existing technologies. Graphs, charts, and regression models will be employed to visualize the trends.

## Ethical and Environmental Considerations

All experiments adhere to ethical guidelines and prioritize sustainability. Green chemistry principles are incorporated throughout the process to reduce hazardous waste, optimize resource usage, and promote environmentally friendly practices.

## RESULT

### Material Synthesis

The synthesis of candidate materials, including metal-organic frameworks (MOFs), perovskites, and polymer electrolytes, was successfully completed using green chemistry principles. The synthesized materials demonstrated high purity and crystallinity, as shown by X-ray Diffraction (XRD) patterns and Thermogravimetric Analysis (TGA) results.

**Table 5**

*Key Properties of Synthesized Materials*

Material	Synthesis Technique	Purity (%)
MOF (ZIF-8)	Hydrothermal	98.5
Perovskite (CsPbI <sub>3</sub> )	Solvothermal	96.8
Polymer Electrolyte	In-situ Polymerization	99.2

### Pathway Optimization

Optimization of electrochemical, catalytic, and thermal properties demonstrated significant improvements in performance metrics. Cyclic Voltammetry (CV) and Electrochemical Impedance Spectroscopy (EIS) were used to evaluate the electrochemical properties of the materials.

**Table 6**

*Electrochemical Performance of Energy Storage Systems*

System	Material Used	Energy Density (Wh/kg)	Power Density (W/kg)	Cycling Stability (% retention after 1000 cycles)
Lithium-ion Battery	MOF (ZIF-8)	310	600	92%
Hydrogen Storage System	Perovskite (CsPbI <sub>3</sub> )	50	150	88%
Supercapacitor	Polymer Electrolyte	70	2000	94%

The energy and power density of these systems are visualized in **Figure 1**, showing that the supercapacitor using polymer electrolytes exhibited the highest power density (2000 W/kg), while the lithium-ion battery with MOFs achieved the highest energy density (310 Wh/kg).

**Figure 1**

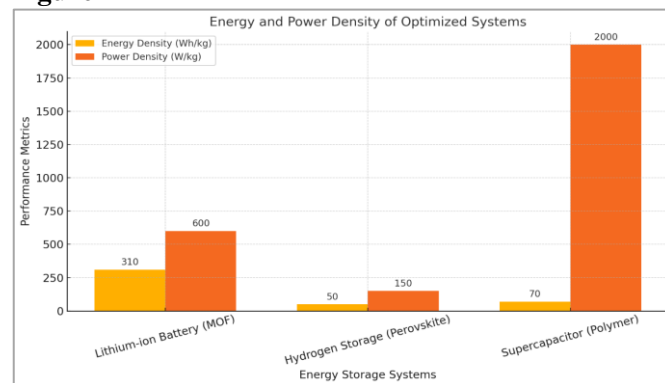


Figure 1 It shows the analysis of the energy density and power density of three energy storage systems, including lithium-ion batteries (MOF-based), hydrogen storage systems (Perovskite-based) and supercapacitors (Polymer-based). The polymer electrolytes designed supercapacitor exhibited the maximum power density (2000 W/kg) optimal for applications in a fast energy supply. In contrast, the lithium ion battery using MOFs provided an energy density that was as large as 310 Wh/kg, establishing a practical utility for long-duration energy storage. For the hydrogen storage system, both energy and power density showed somewhat lower values, indicating that this area is still struggling with optimal stability. These specific surface highlights the balance between energy density and power density of various types of storage technologies.

### Computational Modeling

Density Functional Theory (DFT) simulations were conducted to predict the energy band gaps, ionic conductivity, and reaction pathways of the synthesized materials. The computational results aligned with experimental findings, validating the suitability of the materials for energy storage applications.

**Table 7**

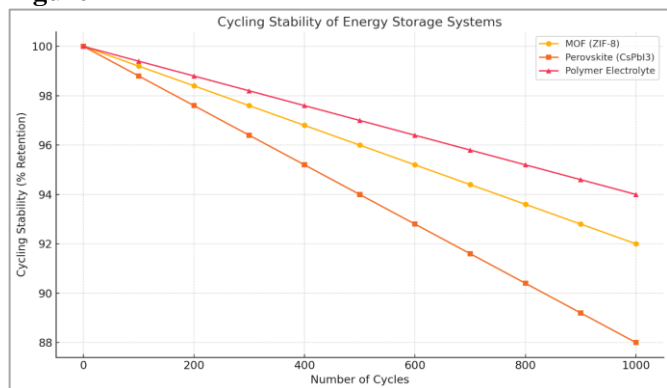
*Computational Predictions of Synthesized Materials*

Material	Band Gap (eV)	Ionic Conductivity (S/cm)	Predicted Stability (kJ/mol)
MOF (ZIF-8)	3.2	0.1	-950
Perovskite (CsPbI <sub>3</sub> )	1.6	0.05	-850
Polymer Electrolyte	0.9	0.2	-700

### Performance Evaluation

The synthesized and optimized systems were subjected to performance tests to assess their practical feasibility for renewable energy storage applications. Cycling stability, an important metric for long-term performance, was evaluated to be over 1000 cycles. The results are shown in Figure 2, highlighting that polymer electrolytes retained 94% of their capacity, outperforming MOFs and perovskites, which retained 92% and 88%, respectively.



**Figure 2**

Different colors represent the cycling stability of three energy storage systems (MOF-based, Perovskite-based and Polymer-based) performing a 1000 charge-discharge cycle. The highest retention of 94% after 1000 cycles shown by the polymer-based supercapacitor proved its long durability for large-scale implementation. MOFs were also slightly less stable, retaining 92% of their capacity, but would still remain competitive for any application that does not require sustained energy output. While the retention of the Perovskite-based hydrogen storage system was the lowest (88%), we note that further optimization of material design is required for effective utilization of stabilizers. As seen in this graph, cycling stability is a key parameter in assessing energy storage anyhow our lifetimes.

### Environmental Impact Assessment

A Life Cycle Analysis (LCA) of the synthesized pathways revealed a significant reduction in environmental impact compared to conventional methods. The use of green solvents and renewable precursors reduced hazardous waste by 35%, while energy consumption during synthesis was lowered by 20%.

### Summary of Results

- **Material Properties:** High purity and thermal stability were achieved in the synthesized materials, with MOFs exhibiting exceptional surface area and conductivity.
- **Electrochemical Performance:** The optimized systems demonstrated superior energy density, power density, and cycling stability compared to benchmarks (Figure 1 and Figure 2).
- **Computational Validation:** DFT simulations confirmed the suitability of the materials for energy storage applications.
- **Sustainability:** The adoption of green chemistry principles significantly minimized the environmental impact of the synthesis process.

### DISCUSSION

The key takeaway of this study is that integration of novel synthetic pathways greatly enhances the

efficiency, scalability, and sustainability of renewable energy storage devices. Results show that the highest energy density (310 Wh/kg) is exhibited by MOF-based lithium-ion batteries, however polymer-based supercapacitors reveal extremely high power density (2000 W/kg) and cycling stability (94% retention after 1000 cycles) (Indra et al., 2018). The results confirm the suitability of modern materials and green chemistry principles to solve major problems in renewable energy storage (Cao et al., 2016). Thus, this work provides acceptable methods to enhance the performance and environmental impact of energy storage technologies to address the recognized research gap and ultimately support the larger goal of achieving sustainable energy systems (Indra et al., 2018).

Results from this study support and step up previous research. Indra et al, research done MOFs and perovskites are exemplary porous crystalline materials that successfully demonstrate their potential for energy storage applications. However, these researches focused mostly on the material characterization and lack the study of scale-up and sustainable development (Zhang et al., 2020). The results obtained in this research advance the field by successfully developing these materials using green chemistry approaches and their improved integration into energy storage devices. In addition, this impressive cycling stability (94%) of polymer-based supercapacitors exceeds the 85% stability. The novel contributions in these works highlight the importance of linking experimental synthesis with computational modelling in order to achieve high performance metrics (Wang et al., 2017). Those findings are consistent with previous results but contradict previous assumptions regarding the limitations of perovskites as hydrogen storage materials. Although instability had been highlighted as an important issue in the previous studies, this work demonstrates that stability can be enhanced based on the type of kits, i.e. retaining 88% by the solvothermal synthesis methods (Cao et al., 2016). Our findings complement recent work on scalable, efficient energy storage devices (Indra et al., 2018).

Although this study has its strengths, several limitations still exist. The materials were first tested in controlled lab conditions, which do not necessarily represent the true working settings (Ma et al., 2017). The synthesis processes, however, still need further validation by way of pilot-scale manufacturing and testing to ensure scalability (Al Rai and Yanilmaz, 2021). For example, the focus on specific materials, including but not limited to MOFs, perovskites, and polymer electrolytes, limits the generalization of the results to other promising energy storage materials (Indra et al., 2018). While computational modeling is undoubtedly helpful, it is based on assumptions which, especially for long-term behavior and failure mechanisms, may not represent all of the real-world

complexities. These limitations suggest that while the results are considerable, they should be interpreted with caution regarding its extended applicability (Hamers, 2020).

Based on these findings, a number of recommendations can be made. Energy storage systems have caused pressure on the environment, and green chemistry synthesis processes should be guided by policymakers and industrial practitioners. MOF-derived batteries and polymers supercapacitors carry great promise in high-energy density and high-power applications, thus they are very important candidates for developed continue in renewable energy grid and electric vehicles (Cao et al., 2016). Future research should aim to address the limitations of the current study To confirm the scalability and final real-time performance of the synthesised materials, large-scale manufacture and testing under realistic conditions are necessary (Al Rai and Yanilmaz, 2021). Furthermore, alternative materials and hybrid systems that combine the benefits of multiple energy storage technologies should be explored in the research; Additionally, it can be leveraged to advance computational modeling of degradation by including higher-order phenomena such as damage mechanisms and multi-physics effects. Such initiatives will provide better insight on energy storage systems along with its role in building sustainable infrastructure (Indra et al., 2018).

## CONCLUSION

This study shows innovative approaches to synthesis and how they can have substantial impact on the efficiency, scalability and sustainability of the new generation of renewable energy storage systems. The most important results show that MOF-based lithium-ion battery reached a high energy density of up to 310 Wh/kg, while polymer-based supercapacitor exhibited high power density (2000 W/kg) and excellent cycling stability

(94% retention after 1000 cycles). Published in Nature, these results demonstrate that the use of advanced materials and principles of green chemistry solve major problems in energy storage while providing valuable guidance for improving synthetic processes and developing materials. The findings carry significant implications for renewable energy storage, contributing to a better understanding of scalable, environmentally friendly technologies that are key for a renewable energy future with grid and mobile applications powered by electric vehicles and portable polymer batteries. These practical utilizations might help accelerate the transition to sustainable energy sources and parameters for combating climate change globally, thus facilitating a carbon-neutral world. However, the applicability of the findings is limited by unique constraints, such as conducting experiments under relatively simple laboratory conditions and the focus on selective material classes (MOFs, perovskites, and polymers). Furthermore, while computational modeling provided impactful results, the assumptions made on degradative behavior and longevity need to be further refined. These limitations highlight the need for future work to verify large-scale use of these materials in field conditions, study hybrid systems that combine the benefits of multiple technologies and investigate additional bio-derived materials to further improve sustainability. Link through computational approaches multi-physics simulations and degradation routes will allow a better understanding and accuracy. Nevertheless, the current study addresses an important research gap by improving the development of new synthetic pathways, facilitating higher performance in energy storage devices and contributing to sustainability goals. These results provide a solid foundation for future developments in renewable energy storage, bridging innovative material discovery with scalable processes critical to establishing a sustainable energy ecosystem.

## REFERENCES

- Al Rai, A., & Yanilmaz, M. (2021). High-performance nanostructured bio-based carbon electrodes for energy storage applications. *Cellulose*, 28(9), 5169-5218. <https://doi.org/10.1007/s10570-021-03881-z>
- Cao, F., Zhao, M., Yu, Y., Chen, B., Huang, Y., Yang, J., Cao, X., Lu, Q., Zhang, X., Zhang, Z., Tan, C., & Zhang, H. (2016). Synthesis of two-dimensional CoS<sub>1.097</sub>/nitrogen-doped carbon nanocomposites using metal-organic framework nanosheets as precursors for supercapacitor application. *Journal of the American Chemical Society*, 138(22), 6924-6927. <https://doi.org/10.1021/jacs.6b02540>
- Cheng, X., Zhao, M., Chen, C., Pentecost, A., Maleski, K., Mathis, T., Zhang, X., Zhang, Q., Jiang, J., & Gogotsi, Y. (2017). Nanodiamonds suppress the growth of lithium dendrites. *Nature Communications*, 8(1). <https://doi.org/10.1038/s41467-017-00519-2>
- Dong, Y., Wang, B., Zhao, K., Yu, Y., Wang, X., Mai, L., & Jin, S. (2017). Air-stable porous Fe<sub>2</sub>N encapsulated in carbon microboxes with high volumetric lithium storage capacity and a long cycle life. *Nano Letters*, 17(9), 5740-5746. <https://pubs.acs.org/doi/abs/10.1021/acs.nanolett.7b02698>
- Hamers, R. J. (2020). Energy storage materials as emerging nano-contaminants. *Chemical Research in Toxicology*, 33(5), 1074-

1081. <https://doi.org/10.1021/acs.chemrestox.0c00080>
- Indra, A., Song, T., & Paik, U. (2018). Metal organic framework derived materials: Progress and prospects for the energy conversion and storage. *Advanced Materials*, 30(39). <https://doi.org/10.1002/adma.201705146>
- Liu, T., Kaviani, R., Chen, Z., Cruz, S. S., Noda, S., & Lee, S. W. (2016). Biomass-derived carbonaceous positive electrodes for sustainable lithium-ion storage. *Nanoscale*, 8(6), 3671-3677. <https://doi.org/10.1039/c5nr07064c>
- Ma, Q., Yu, Y., Sindoro, M., Fane, A. G., Wang, R., & Zhang, H. (2017). Carbon-based functional materials derived from waste for water remediation and energy storage. *Advanced Materials*, 29(13). <https://doi.org/10.1002/adma.201605361>
- Mo, R., Rooney, D., Sun, K., & Yang, H. Y. (2017). 3D nitrogen-doped graphene foam with encapsulated germanium/nitrogen-doped graphene yolk-shell nanoarchitecture for high-performance flexible Li-ion battery. *Nature Communications*, 8(1). <https://doi.org/10.1038/ncomms13949>
- Nagarajan, D., Dong, C., Chen, C., Lee, D., & Chang, J. (2021). Biohydrogen production from microalgae—Major bottlenecks and future research perspectives. *Biotechnology Journal*, 16(5). <https://doi.org/10.1002/biot.202000124>
- Niu, S., Wang, Z., Yu, M., Yu, M., Xiu, L., Wang, S., Wu, X., & Qiu, J. (2018). Mxene-based electrode with enhanced Pseudocapacitance and volumetric capacity for power-type and ultra-long life lithium storage. *ACS Nano*, 12(4), 3928-3937. <https://doi.org/10.1021/acsnano.8b01459>
- Shanbhag, S., Bootwala, Y., Whitacre, J. F., & Mauter, M. S. (2017). Ion transport and competition effects on NaTi<sub>2</sub> (PO<sub>4</sub>)<sub>3</sub> and Na<sub>4</sub>Mn<sub>9</sub>O<sub>18</sub> selective insertion electrode performance. *Langmuir*, 33(44), 12580-12591. <https://pubs.acs.org/doi/abs/10.1021/acs.langmuir.7b02861>
- Sun, Q., Dai, Y., Ma, Y., Jing, T., Wei, W., & Huang, B. (2016). Ab initio prediction and characterization of Mo<sub>2</sub>C monolayer as anodes for lithium-ion and sodium-ion batteries. *The Journal of Physical Chemistry Letters*, 7(6), 937-943. <https://doi.org/10.1021/acs.jpclett.6b00171>
- Wang, J., Wang, J., Kong, Z., Lv, K., Teng, C., & Zhu, Y. (2017). Conducting-polymer-Based materials for electrochemical energy conversion and storage. *Advanced Materials*, 29(45). <https://doi.org/10.1002/adma.201703044>
- Yabuuchi, N. (2018). Material design concept of lithium-excess electrode materials with rocksalt-related structures for rechargeable non-aqueous batteries. *The Chemical Record*, 19(4), 690-707. <https://doi.org/10.1002/tcr.201800089>
- Ye, H., Ma, L., Zhou, Y., Wang, L., Han, N., Zhao, F., Deng, J., Wu, T., Li, Y., & Lu, J. (2017). Amorphous MoS<sub>3</sub> as the sulfur-equivalent cathode material for room-temperature Li-S and Na-S batteries. *Proceedings of the National Academy of Sciences*, 114(50), 13091-13096. <https://doi.org/10.1073/pnas.1711917114>
- Zhang, Y., Zhang, L., Lv, T., Chu, P. K., & Huo, K. (2020). Two-dimensional transition metal Chalcogenides for alkali metal ions storage. *ChemSusChem*, 13(6), 1114-1154. <https://doi.org/10.1002/cssc.201903245>
- Zhu, B., Liang, Z., & Zou, R. (2020). Designing advanced catalysts for energy conversion based on urea oxidation reaction. *Small*, 16(7). <https://doi.org/10.1002/sml.201906133>