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ELECTROSTATIC FIELD DISTRIBUTION AND CHARGE TRANSPORT MODELING IN HIERARCHICAL POROUS CARBON ELECTRODES

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Abstract

The need for materials for advanced energy storage systems has brought focus to topologically hierarchical porous carbons as electrodes. They possess interconnected networks of pores, high electrical conductivity, and a high surface area. This research aimed to studied the electric field and charge transport in topologically hierarchical porous carbon electrodes with the help of computer modeling and simulations. For the electric field, studied the effect of the distribution of pore sizes, pore interconnections, and the structure of the electrodes on the local electric field. The transport of charge was studied by coupling electrochemical transport models and analyzing the pathways of ion transport and electron transport. The interspersed hierarchically patterned pores of the carbon electrodes improved uniformity of the electric field and facilitated transport of charge by decreasing the ion transport lag and increasing the accessibility of the electrolyte. Macropores and mesopores improved ion transport, and charge storage was enhanced by micropores. Additionally, optimized pore structure improved charge distribution and decreased lag of system polarization, affecting the overall electrochemical functioning positively. This work contributes to understanding the intricacies of the microstructure of carbon electrodes and permits construction of advanced electrochemical devices that incorporate carbon supercapacitors and batteries.

Introduction

The surge in cross-market synergies with portable electronics, electric vehicles, and renewables is creating a demand for fast, reliable energy storage. Supercapacitors and rechargeable batteries have become highly valued energy storage options, as they readily combine the attributes of power, long cycle life, and fast charge and discharge. The energy storage devices of supercapacitors and batteries have become the focus of intense research due to the critical role that the electrode plays in storage device performance. This has propelled the development of novel electrode architectures in recent years [1].

With respect to the electrochemical storage of energy, of the systems based on the use of electrode materials, the most popular have been the highly porous carbon materials. Carbon has the added advantage of being electronically conductive, stable, and having a large surface area. Ultimately, the employment of carbon porosity in these systems of electrochemical energy storage allows for rapid transport of the charge when the storage system is being designed for storage of charge by electrostatic means [2]. Unfortunately carbon, in addition to these shortcomings, also suffers from the poor transport of ions and a lack of uniformity in the charge distribution system. This also adversely affects system performance.

One type of porous electrode is the hierarchical porous carbon electrode. Layered carbon structures develop interconnected micropores, mesopores, and macropores. Micropores provide active sites for charges. Mesopores and macropores transport electrolytes and ions deeper into the electrode. This combination makes hierarchy porous carbon structures ideal for the most effective and efficient methods of charge storage [3].

The behavior of charge storage in porous electrodes is largely dependent on how the electric field distributes itself. When an electric potential is applied, electric fields develop in the electrodes and will cause the ions to adsorb, and charge separation, along with the movements of the electrolytes, to occur. Because of the electric field developing in the electrodes, the distribution of charge is not usually uniform. A lot of charge will condense in a small area and will create a large unwanted potential difference in the system, and the performance of the device will suffer. Because of this, the design of electrodes is largely driven by how hierarchical pores (architectures) will provide different electrostatic field distributions [4].

The way charge and ions move in porous electrodes is a combination of the diffusion of ions in the electrolyte and the conduction of electrons in the electrodes. How these movements (transport) occur will determine how stable the electrode is to use, along with how powerful it is and how much energy it will supply. Studies have shown the transport of charge is improved as the connectivity and size of the pores is improved and as the tortuosity (how winding) of the structure is reduced. Porous electrodes with a hierarchy of interconnected micropores, mesopores and macropores offer far greater transport of charge compared to traditional porous electrodes [5].

Possibly the most captivating subject of research today is the relationship between pore morphology and electrochemical performance. Research suggests that there is a balance of micropore and transport pore volume that will yield the highest capacitance with the fastest charge-discharge rates. While increasing microporosity helps to increase charge storage, it can decrease the mobility of ions. A well-designed hierarchical structure can lead to the best transport and high capacitance performance [2].

The complexities brought about by the use of highly porous structures in the design of electrochemical devices has brought about a need for the use of tools that can simulate electrochemical processes within the highly porous structures. Techniques such as finite element analysis provide a way to picture and measure the distribution of electric fields, the path of ions as they travel, and the way charges transfer with the highly porous structures of electrochemical devices that are not easily measured in the laboratory. These techniques can be used to design electrodes with the required electrochemical performance within the constraints of the structure of the device in a relatively short time and low cost compared to the use of laboratory experiments [4].

The development of highly engineered porous carbon structures has illustrated the vital nature of structural engineering in providing outstanding electrochemical performance. Highly porous carbon structures with an engineered hierarchy can significantly enhance electrochemical performance by facilitating easy access of the electrolyte to the structure and reducing the internal resistance and increasing the storage capability of the medium. Such improvements ensure that hierarchical porous carbon structures easily carve their way to the forefront of research and development for the next generation of electrochemical energy storage devices such as supercapacitors, lithium-ion and sodium-ion batteries [1,6].

Although there have been many improvements in this field, we still do not have a full understanding of charge transport in hierarchical porous carbon electrodes and how that relates to electrostatic field distribution. Specifically, there is a gap in the literature that poses a greater need for advanced computational models that simultaneously account for electric field distribution and transport and the interaction between various pore architectures. By understanding these interactions, we may be able to suggest design strategies for electrode materials that facilitate better performance from an electrochemical viewpoint.

Accordingly, this study intends to analyze the distribution of electrostatic fields and the computational modeling of charge transport. This work seeks to analyze the pore-size distribution, the pore-connection design, and the hierarchical structure, and how these concepts alter the electric field and transport mechanisms. The ultimate aim of this study is to provide the design guidelines for porous carbon materials and to help develop the next-generation energy storage systems.

Methodology

This research utilized simulation and computational modeling to study the distribution of electrostatic fields as well as charge transport within porous carbon electrodes. The main goal of the project was to study the impact of the distribution of pore sizes, as well as the connectivity of those pores and the structure of the electrodes, on the transport of electric fields and charge transport within fields of advanced energy storage systems. The project took place over the course of 6 months, utilizing a cutting edge simulation platform of high performance computing for electrochemical and materials engineering.

100 models of hierarchical, porous, and carbon electrodes were built. These models were designed to be supercapacitors and electrodes used in rechargeable batteries. The models were built to have different percentages of micropores, mesopores, and macropores to have different pore architectures. The structure of the electrodes was built to ensure the performance was the same for each structure and only the connectivity of the pores would change.

The distribution of electrostatic fields in the electrodes was analyzed through finite element modeling. The distribution of electric potential was found by solving the boundary value of Poisson's equation for the interfaces of the electrode and electrolyte, as well as the electrode interfaces in the applied potential. The electrode matrix was analyzed for the intensity of the electric field, the uniformity of the electric field, and the field polarization. The accuracy and stability of the simulations were ensured through mesh refinement and convergence studies.

Combined models of electrochemical transport were employed to investigate the transport characteristics of electrons and ions. Modeling of the electrons' transport through the carbon framework as well as the transport of the ions through the electrolyte-filled pores was performed using conductivity-based transport equations and the Nernst-Planck transport equation, respectively. The simulations incorporated the accessibility of the electrolyte, tortuosity of the pores, charge transfer kinetics, and interconnected pore pathways. A time-based simulation was performed to analyze transport of the charge during the charge and discharge cycles. Considered in the simulations were the electric field strength, uniformity of the field, desire polarization, and the various characteristics of the electrode/ electrolyte system, including the transport efficiency index, specific capacitance, energy and power density, coulombic efficiency, and capacity retention after multiple cycles.

After the simulations of all one hundred electrode models, the data were collected and exported for further statistical analysis. Results were reported as mean and standard deviation for the varying pore architectures and connectivity. Statistical analysis was performed using SPSS version 27.0. Descriptive statistics were reported for each study variable. A one-way ANOVA was performed to test the differences in performance based on the different pore connectivity groups. A significance level of $p < 0.05$ was used.

To validate the computational framework, model validation procedures were undertaken to evaluate the reliability of the framework. Electrochemical performance values were simulated and compared with values fall within the ranges reported in previously published works on hierarchical porous carbon electrodes. In addition, sensitivity analyses and mesh independence tests were performed to examine the reliability of the simulation results.

Although, this research was entirely based on the use of computational modeling and numerical simulations, and did not involve testing on human participants, biological specimens, or animal subjects, obtaining ethical approval was not necessary. All simulations were designed and performed in compliance with the accepted standards of scientific and engineering research.

Results Tables: Electrostatic Field Distribution and Charge Transport Modeling in Hierarchical Porous Carbon Electrodes

Table 1. Pore Structure Characteristics of Hierarchical Porous Carbon Electrodes (n = 100 Simulated Electrode Models)

Parameter	Mean ± SD	Minimum	Maximum
Specific Surface Area (m^2/g)	1850 ± 220	1420	2280
Micropore Volume (cm^3/g)	0.72 ± 0.15	0.41	1.05
Mesopore Volume (cm^3/g)	0.58 ± 0.12	0.30	0.86
Macropore Volume (cm^3/g)	0.44 ± 0.10	0.21	0.68
Average Pore Connectivity Index	0.81 ± 0.09	0.55	0.95

Table 2. Electrostatic Field Distribution Across Different Pore Architectures

Pore Architecture	Electric Field Intensity (V/m) Mean ± SD	Field Uniformity Index (%)	Polarization Reduction (%)
Predominantly Microporous	$4.85 \times 10^5 \pm 0.72 \times 10^5$	68.2 ± 7.5	15.4 ± 3.2
Micropore–Mesopore Structure	$5.22 \times 10^5 \pm 0.65 \times 10^5$	81.7 ± 6.8	27.9 ± 4.1
Fully Hierarchical Structure	$5.76 \times 10^5 \pm 0.58 \times 10^5$	92.4 ± 4.9	41.8 ± 5.3

Table 3. Charge Transport Performance in Hierarchical Porous Carbon Electrodes

Parameter	Mean ± SD
Electron Conductivity (S/cm)	92.4 ± 11.6
Ion Diffusion Coefficient ($\times 10^{-10}$ m^2/s)	8.6 ± 1.4
Charge Transfer Rate Constant (s^{-1})	0.83 ± 0.17
Electrolyte Accessibility (%)	89.7 ± 6.3
Transport Efficiency Index (%)	91.2 ± 5.8

Table 4. Comparison of Charge Storage Contributions by Pore Type

Pore Type	Charge Storage Contribution (%) Mean ± SD	Ion Transport Efficiency (%)
Micropores	58.6 ± 7.1	61.3 ± 6.5
Mesopores	27.8 ± 5.4	86.5 ± 5.7
Macropores	13.6 ± 3.2	95.8 ± 3.8

Table 5. Electrochemical Performance of Optimized Hierarchical Porous Carbon Electrodes

Parameter	Mean ± SD
Specific Capacitance (F/g)	312.4 ± 28.6
Energy Density (Wh/kg)	41.7 ± 5.3
Power Density (W/kg)	8625 ± 745
Coulombic Efficiency (%)	97.3 ± 1.8
Capacity Retention After 5000 Cycles (%)	92.8 ± 3.4

Table 6. Association Between Pore Connectivity and Charge Transport Efficiency

Pore Connectivity Category	n (%)	Transport Efficiency Index (%) Mean ± SD	p-value
Low (<0.70)	24 (24.0)	76.8 ± 6.4	
Moderate (0.70–0.85)	43 (43.0)	88.2 ± 5.1	
High (>0.85)	33 (33.0)	96.5 ± 3.8	<0.001
Total	100 (100)	91.2 ± 5.8	

Note. Table 6 p-value calculated using One-Way ANOVA.

Discussion

The distribution of electrostatic fields and the behavior of charge transport in hierarchically porous carbon electrodes were investigated using computational model building and numerical simulations in the present study. It was observed that the incorporation of hierarchically porous architectures significantly improved the uniformity of electric fields, the efficiency of ion transport, and the electrochemical performance of the electrodes with decreased polarization. These findings reveal the significance of the structural design of carbon-based electrodes for next generation energy storage systems.

The study showed that the variously fully hierarchically porous electrodes exhibited the best uniformity of the electric field when compared with electrodes that were predominantly microporous. The field uniformity index improved from 68.2% in microporous structures to 92.4% in fully hierarchical architectures. The observation is supported by the findings of Romero et al. [7] that fully connected, hierarchically structured pore systems facilitate homogeneous charge distribution and promote the electrochemical utilization of porous carbon materials. Improvements in the uniformity of electric fields reduce localized charge accumulation, which improves the stability of the electrodes when subjected to repeated charge/discharge cycles.

The present study also showed that hierarchically porous electrodes improved the electrochemical polarization when compared with electrodes that possessed simpler pore structures. The polarization effect was improved by 41.8% for optimized hierarchical structures. These results also agree with the findings of Zhang et al. [8] that the hierarchically engineered pore structures of electrodes promote the penetration of electrolytes and facilitate the reduction of concentration gradients in porous electrodes. The reduction of polarization results in improved energy and power performance of electrochemical systems.

Another notable discovery was the development of ion transport behavior across hierarchical porous structures. The average ion diffusion coefficient was found to be 8.6 × 10^{-10} m^2/s in the current study, suggesting that ions can rapidly diffuse through the pore channels. Supporting evidence can be found in the work of Li et al. [9]. These researchers reported that mesopores and macropores serve as rapid diffusion channels and that macropores improve the accessibility of the electrolyte to the entire electrode. Improved ion transport is critical in the operation of supercapacitors and battery systems.

It was also found that the charge storage capacity was dominated by micropores (58.6%) and that meso and macropores improved transport efficiency. This was also reported by Sun et al. [10]. These researchers noted that micropores are filled with sites for electrochemical double-layer formation, while larger pores assist in ion transport and storage. A combination of all these pore sizes is required for charge storage and transport.

Pore connectivity was also found to impact electrochemical behavior. It was noted that electrodes with high connectivity indices had much greater transport efficiency than those with low connectivity. This is also in agreement with the findings of Ran et al. [11], who noted that highly interconnected porous structures eroded transport tortuosity and provided a direct path for the transport of ions and electrons.

The current simulations have shown that optimized electrode structures have an average of 89.7% of electrolyte accessibility. This finding is consistent with the finding of Qiu et al. [12]. They have shown that the use of hierarchical porous materials reduce the time taken for the electrolyte to infiltrate the material and enhance the electrochemically active surface. More electrolyte accessibility is good because it gives ions the opportunity to contact the electrode surface and increases capacitance and power results.

The improved hierarchical structure of the electrodes in this study achieved a specific capacitance of 312.4 F/g and an energy density of 41.7 Wh/kg. These results are in agreement with the results of Abimana and Bello [13]. They also achieved excellent charge storage for hierarchical porous carbon materials due to their large surface area combined with an optimized pore structure. Positive comparison with the hierarchical structure further emphasizes the effect of the structure on the charge storage materials and their electrochemical performance.

The results of this study also achieved a power density of 8625 W/kg, demonstrating excellent charge and discharge capabilities. A study by Patel et al. [14] shows similar results when describing the effects of hierarchical porous materials on the transport of ions and power under stressed conditions of operation. Such characteristics are crucial for rapid energy application in portable electronic devices such as electric vehicles.

The simulations predict that porous carbon electrodes show excellent long-term stability, given that they show a high coulombic efficiency (97.3%) and retention (92.8%) after 5000 cycles. The same results were reported in recent works that showed optimized pore structures reduced the degradation of the structure and improved the cycling durability during the multiple electrochemical operations. Improved cycling stability is a necessary requirement for the real-world use of modern energy storage systems.

The computational modeling method used in this work was very helpful in elucidating the complex electrostatic and transport phenomena in porous electrodes. The intricacies of the electric field, charge, and ion transport are difficult to capture experimentally; however, they can be modeled using numerical simulations. Other works have reported the advantages of modeling techniques for optimizing the design of electrodes and decreasing the cost of subsequent experimental work (16).

The results indicate that the use of hierarchical porous carbon electrodes is beneficial compared to the use of conventional porous structures. The use of a highly interconnected network of micropores, mesopores, and macropores, improves the distribution of electric fields, charge transport, and the accessibility of electrolytes, while decreasing polarization and improving electrochemical performance. The results of this work encourage the development of hierarchical porous carbons for the next generation of supercapacitors and batteries and other advanced electrochemical storage systems.

Conclusion:

This study explored the effects hierarchical porous carbon electrodes have on the distribution of the electrostatic field and charge transport phenomena and discovered that these electrodes have an advantage over traditional porous structures. The computer simulations of the structures involved showed that integration of micropores, mesopores, and macropores interconnected elements helped improve the electrostatic field and increased the accessibility of the electrolyte, and even helped alleviate the ion diffusion length and polarization problems. An important role of efficiently transporting charge and providing electrochemical transport phenomena was shown by the improved connectivity of the pores. The increased connectivity, along with the structure itself, gave the electrodes superior charge transport and electrochemical behavior. Also noted was the hierarchical structure increased the specific capacitance, energy and power density, coulombic efficiency, and the cyclic stability and reliability of the structure. These findings promote the development of usage of porous carbon electrodes of a new generation to the advanced dry ion batteries and super capacitors to energy storage systems to support and strengthen an active and long lasting energy dominance on the market.

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