Programa de Doctorat Eletroquímica.

PLA DE RECERCA

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Línia de recerca:

Títol de la Tesi: Double-carbon structure energy storage device

El projecte ha de constar de les següents parts:

1. Introducció: interès del tema
2. Objectius
3. Pla de treball i cronograma.
4. Bibliografia

Màxim 1200 paraules (sense comptar la bibliografia)

1. INTRODUCTION

Increased energy consumption along with the progress in the economic development brought severe pollution which was a serious threat to human health and environment security. The paradox between the dependence on energy of human being and the combustion of fossil fuels motivates the development of utilization of various energies, such as solar energy, wind energy, tidal energy, and nuclear energy. Therefore, the storage of different types of energy became a key issue[1, 2]. To evaluate the most relevant storage solution, it is necessary to consider the lifetime, reliability, storage capacity, cost, and environmental impact. Implementing the efficient and economic energy storage in the power infrastructure can bring great benefits to the power industry and human beings. According to the final energy, there are electric energy storage and non-electric energy storage. Electric energy storage systems accept and return the stored energy as electric power, although they may store the energy in another form[3, 4]. Supercapacitor and battery, as two main electric energy storage systems, have been widely applied in different fields ranging from portable electric devices to smart grid[5]. Compared with battery, supercapacitor possesses high power density and long cycle life (100000 cycles) which ensure the fast charging/ discharging speed and almost no maintenance charge[1].

Beyond trying to find the optimum cation to be moved between an anode and a cathode, an alternative is to take advantage of two ions, an anion and a cation that are inserted/extracted in/from the cathode and anode to charge/discharge the battery. This type of energy storage system is known as dual-ion battery (DIB). In dual-ion batteries we could use a carbon-based electrode. The advantage of DIBs are much higher voltages of 4.0 V and above, energy densities and cycle stabilities[6]. An important additional advantage of DIBS is that they can be environmental friendly, easy to recycle and low cost[7, 8]. Previous studies have shown that the theoretical specific capacity of anion intercalated/deintercalated graphite is about 120 mAh/g, which indicates that the energy density of DCBs can reach 240 Wh/kg. However, due

to its expensive ionic salt and harsh preparation methods, it is currently difficult to apply it on a large scale.

Electrochemical capacitors, so-called supercapacitors (SCs), are electrochemical energy-storage devices which can provide higher power density than batteries and higher energy density than conventional dielectric capacitors. Supercapacitors possess great advantages, especially in terms of rapid charge and discharge and highly prolonged cycle life[9]. Generally, the mechanism of energy storage for SCs can be explained using three types of capacitive behaviors: (1) electrochemical double layer capacitors (EDLCs) use the electric charge that accumulates at the electrode interface, (2) pseudo-capacitance (PC) develops from quick and reversible surface redox processes, and (3) hybrid capacitors (HSCs) take advantage of both mechanisms[10].

However, they may suffer from low energy density compared to batteries. With the advantages of micro-size and lightweight, supercapacitor can be used as power supplies for various portable electric devices like smart phone, notebook, etc. In hybrid electric vehicles, supercapacitor can meet the requirements of high power output for the short-term acceleration and high capacity for temporary energy storage equipment during braking, which save energy and avoid batteries suffering high frequency fast charge/ discharge cycles. In this case, supercapacitor is acting as a bridge for power/energy difference between high power output (capacitor) and high energy storage (batteries) and has the potential to play an important role in future large-scale hybrid energy systems[9].

A double-carbon structure energy storage device (DCESD) is an energy storage device in which both anode and cathode materials use carbon materials. With the rise of DIBs, there are many possibilities for DCESD. On the one hand, most of the current electrode/batteries type HSCs are designed with battery materials for the negative electrode and active carbon for the positive electrode, and HSCs with Na/K-organic electrolyte have a voltage range from 0 to 4.2 V. The energy density of such capacitors is close to but difficult to reaches 80 Wh/kg. However, the recent emergence of DIBs gives us new hope if we use graphitized microcrystalline activated carbon as the cathode material for DCESD and add additional capacity by intercalating graphitized structures with anions (e.g., ClO_4^-, PF_6^-, $TFSI^-$); at the same time, the anion intercalated graphite has a higher potential, which can potentially increase the operating voltage of DCESD and further enhance the energy density of DCESD on line[11]. On the other hand, carbon material has good environmental friendly characteristics, abundant resources, easy to recycle, good electrical conductivity, controllable layer spacing, and diversity, is a very ideal material for energy storage; through the double-carbon structure of energy storage design, can avoid the use of transition metal elements, to avoid the pollution of some heavy metals, which has great significance for environmental protection and resource conservation[12].

2. OBJECTIVES

The starting hypotheses of the project are the following:

1. An innovative energy storage solution has a huge market and is urgently needed as no current technology provides a solution for the cost-effective implementation of a network of distributed energy storage and for the electric transportation, what is already delaying the deployment of renewables and of the electric vehicle, with very severe consequences for our health and environment.

2. The required energy storage systems have a low price, are totally safe, have a large energy and power density and a long cycling life. These batteries require low cost materials that are abundant, safe, easily produced, environmental friendly, air stable, non-flammable and non-toxic, and energy storage technologies that at both anode and cathode provide high capacity, reasonable operation voltage, high reversibility and very fast kinetics.

3. In hybrid electric vehicles, supercapacitor can meet the requirements of high power output for the short-term acceleration and high capacity for temporary energy storage equipment during braking, which save energy and avoid batteries suffering high frequency fast charge/ discharge cycles. In this case,

supercapacitor is acting as a bridge for power/energy difference between high power output (capacitor) and high energy storage (batteries) and has the potential to play an important role in future large-scale hybrid energy systems.

4. DCESD offer important advantages over alternative battery technologies, including high energy density and environmental friendliness, with easy recycling and low cost.

5. Carbon-related materials have been regarded as optimum electrode candidates owing to their low and toxicity cost, adjustable interlayer spacing, high ionic conductivity and easy to obtain.

3. RESEARCH PLAN AND TIME SCHEDULE

This is a highly interdisciplinary project that involves various scientific and technological fields, such as organic and inorganic chemistry, physical chemistry, materials science and engineering, device physics, solid state physics and electronic engineering. To address this broad set of fields of action, the project will span 48 months and will be divided into 6 work packages (WP):

WP1. Synthesis high-performance carbon materials as the anode of SIBs or PIBs;
Task 1.1 Synthesis of doping heteroatoms in carbon-based materials.
Task 1.2 Synthesis of carbon materials with special morphology, such as honeycomb, sheet, tube, etc., to explore the effect of carbon material shape on electrochemical performance.

WP2. Development of high-performance graphitized active carbon cathode materials to be applied to HSCs;
***Task* 2.1** Synthesis of active carbon materials with different sp2 content and study the effect of graphite crystallinity on DCESD.
Task 2.2 Graphitized structures active carbon was synthesized by transition metal catalysis, and study of the effect of graphitized structures on DCESD.

WP3. Development of high-voltage and high-adaptability DCESD electrolyte system;
Task 3.1 Development of new polymer electrolyte for DCESD.

WP4. Investigation of the reaction mechanism of DCESD;
In order to better explain the reaction mechanism inside DCESD, theoretical calculation simulation will be used to guide experimental research, such as; DFT, finite element calculation, etc..
Task 4.1. Toward reaching the best voltage window for DCESD. The study of the upper limit voltage of DCBs is limited by the stable upper limit voltage of the electrolyte..
Task 4.2. Gaining insight of the transport mechanism of anion intercalation/adsorption mechanism of cathode material. Improve the rate performance of DCBs from the reaction kinetics of the positive electrode material.

WP5. Development of high-performance DCESD, performance test and pushing of this technology toward the market;
Task 5.1 DCESD prototype fabrication: The designed DCESD will be gradually transformed from a button battery to a large-capacity soft-pack system, and the performance of the material is tested while increasing the capacity.

WP6. Collect and disseminate the experimental results to complete the graduation thesis.

Based on the objectives and technical WPs, eight milestones were identified: This project is planned to take place from October 2021 until the end of May 2024. The chronogram of the project is shown as follows:

WPs	Sep 2021 -Sep 2022		Sep 2022 -Sep 2023		Sep 2023 -Sep 2024	
	Semester 1	Semester 2	Semester 1	Semester 2	Semester 1	Semester 2
WP1.						
WP2						
WP3						
WP4						
WP5						
WP6						

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