AY2016-17 UROP PROJECTS

School of Materials Science & Engineering

PROJECT OFFERED BY
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Developing an Automated Data Analytical Tool to Analyse MALDI-TOF Mass Spectrometry of Fingerprint Data

Project Description:

Mass spectrometry based techniques to analyse fingerprints is an actively developing area especially in the current state of emphasis on national security worldwide. This project deals with the data analysis of MALDI-TOF mass spectrometry spectral of fingerprints dusted using engineered nanoparticles. Mass spectrometry (MS) data from a number of different sample groups has been obtained in the form of ASCII files. Each sample contains three data points, each of which have 5 or more replicates. There are a total of 12 samples in one sample group and there are 8 sample groups involved in the study. This boils down to almost 1500 data files which must be analyzed. Therefore there is a need for preparing an automated tool which can analyze/summarize/compile the data at hand. The tool must perform the following tasks:

- Compile each of the 5 or more replicates into a single worksheet
- Obtain the average of the replicates (neglecting outliers) to derive an average spectrum for each data point
- Obtain an accumulation over the three data points to derive a representative spectrum for each sample
- Analyze samples belonging to the various sample groups within and across each group to obtain characteristic peaks, common peaks, unique peaks, etc.

Key words: Matrix-assisted laser desorption/ionization-Time of Flight (MALDI-TOF) mass spectrometry, data analysis, engineered nanoparticles

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Project Objective

1. Develop a tool (e.g. Excel macro based program) to analyse complex spectral data from mass spectrometry.
2. Analyse data from a number of data groups in terms of:
   - Average spectra
   - Identify characteristic peaks
   - Identity commonly occurring peaks
   - Identify unique sample peaks

Major Tasks

1. To conduct literature review and analyse the pros/cons of existing approaches in similar applications.
2. To develop a tool (could be Microsoft Excel based) which can perform data compilation, data trimming and data analysis.
3. To analyse the data at hand and discover common peaks, characteristic peaks and unique peaks.
4. To produce a manual which simplifies the procedure to use the tool developed.
5. To document the findings into a report and suggest possible improvements to tackle similar sets of data in the future.

In the course of this project, the candidate will learn about nanoparticles synthesis, characterization and the process of fingerprint dusting and collection.

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Nanosized Oxides for Anode of Li-ion batteries

Project Description:

A simple method will be applied by using high-energy ball milling to prepare nanosized oxides as anode materials for lithium ion batteries. By introducing a mall quantity of carbon (graphite), the performance of the anode materials could be largely enhances, which is expected to be comparable with the literature data for the materials by using those complicated wet-chemical synthetic route. This is a relatively simple, cost-effective and scalable approach.

Project Objective:

Nanosized oxides will be synthesized by using a new method developed in the lab, for potential applications as anode of Li-ion batteries. The synthesized oxides will be thoroughly characterized by using XRD, SEM/TEM and electrochemical characterization. The students are expected to learn both fundamentals and practical applications of nanomaterials for energy storage in general and Li-ion batteries in specific.

Major Tasks:

Tasks of the project include literature review and analyzing the problems of the current available methods, learning sample preparation with high energy ball milling, sample characterization with XRD/SEM, device assembling and electrochemical characterization and acting as a team player.

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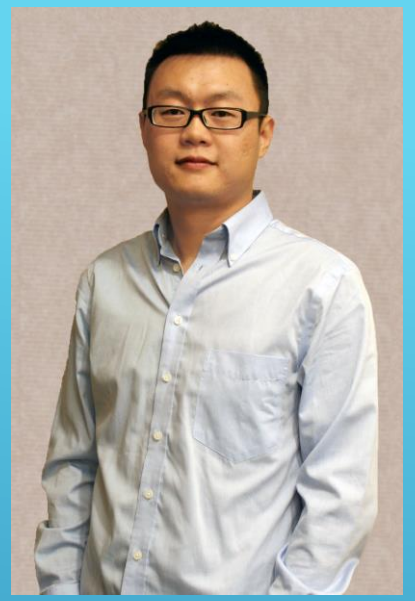

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Metal Oxides Redix Ability and Capacitive Performance

Project Description:

The limited fossil fuel resource and increasing environmental problems have stimulated great interest in sustainable energy resources. To relate the sustainable energy resources to our daily life, efficient energy storage and conversion technologies are highly demanded for smart grid, zero-emission transport, and portable devices. Among these technologies, supercapacitors are a class of attractive energy storage devices due to their high power density, low cost, high safety, and long lifetime. According to the charge storage mechanism, there are two types of supercapacitors. One is the electrical double layer capacitors (EDLCs), which use carbon as electrode materials. EDLCs often give high power density, but low energy density. The other is the pseudocapacitors, which use redox materials like metal oxides and conducting polymers as active electrode materials. Depending on the active materials, pseudocapacitors can achieve fairly high energy density and power density.

Manganese dioxide (MnO_2) is a very popular redox capacitor material and the related research has been intensively conducted in the past few years due to the increasing interest in the field of energy storage and conversion. MnO_2 is a promising electrode material for low cost, high energy density supercapacitors because of its abundance in the earth and high specific energy capacity. MnO_2 is also environmental benign due to its low toxicity. Thus it has a great potential to be widely used in energy devices. The theoretical specific capacitance of MnO_2 is nearly 1400 F/g if all manganese can be involved in the redox reaction (one-electron redox). However, to have all manganese participated in the redox reaction is difficult because the redox reaction happens only at the surface region of MnO_2. It therefore stimulated a great interest to innovate nanosized MnO_2 materials to increase the specific surface area. To date, various methods have been reported to synthesize nanosized MnO_2, including co-precipitation, sol-gel, electro-deposition, hydrothermal, and etc. The use of MnO_2 nanomaterials has given significant improvements in capacitance.

This project will study the redox ability of Mn oxides and correlate this ability with its capacitive performance.

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Project Objective:

The student is expected to learn the knowledge of supercapacitors and the related chemistry and physics. By doing this project, the student will be able to learn how materials determine the performance of an energy storage device like a supercapacitor. The training on the lab skills on chemical synthesis and physical characterizations will be also given to the student.

Major Tasks:

1. To conduct literature review on capacitors and related materials;
2. To learn lab skills on chemical synthesis of oxide materials;
3. To learn the analysis skill on materials characterizations;
4. To analyze the data and correlate materials' properties with the performance.
5. To work as a team member with graduate students.
6. To draw meaningful conclusions using collected data.

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Exploration of Carbonyl-containing compounds as the cathode materials for Li-ion batteries

Project Description:

Electrode materials play a critical role in achieving high energy density and long cycle life Li-ion batteries. The increasing concern with respect to the use of traditional inorganic electrode materials on resources and environmental issues has strongly inspired scientists to search for green energy electrodes. Organic compounds are potentially sustainable and renewable materials as many of them can be obtained from natural products and biomass.

Among all the organic materials, carbonyl-containing compounds are considered as the most promising type of cathode materials attributing to their high working potential, good redox ability and high theoretical capacity. Examples including 1,4,5,8-naphthalenetetracarboxylic dianhydride (NTCDA) and 3,4,9,10-perylenetetracarboxylic dianhydride (PTCDA) have been demonstrated to show good electrochemical performances as active cathode materials.

This project is to explore the possibility of promising carbonyl-containing organic candidates. To achieve different battery performances of the organic materials, one of the strategy is to incorporate carbonyl groups into the organic structures as well as to control the molecular weight of the organic materials. The scope of the project is to select different carbonyl-containing organic structures and compare their battery performances through the fabrication of lithium half cells.

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Project Objective:

The objective of the project is to equip students with the fundamental knowledge related to organic-based rechargeable batteries. At the end of the project, the students should be familiar with the battery performances of several carbonyl-containing organic electrode materials. The detailed objectives are listed below:

1. To understand the fundamental working principle of a typical Li-ion battery.
2. To explore the state-of-the-art carbonyl-containing organic electrode materials, especially the cathode materials.
3. To be familiar with the sample preparation process.
4. To be able to analyse some of the basic electrochemical results of the organic materials.

Major Tasks:

Upon completion of the project, the student(s) is/are:

1. To be able to explain the fundamental working principle of the Li-ion battery.
2. To understand the basic sample preparation process.
3. To know a bit about the current situation of the organic cathode materials.
4. To perform basic analysis of the preliminary experimental results.
5. To provide recommendations with respect to the project.