Research proposal

The Study of Carbon Nanotubes as electrode materials and Metal Coordination complexes as molecular spacers to be used in supercapacitors' applications

The University of North Carolina at Charlotte

by
Nesreen Elathram

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Approved by:

Dr. Jordan C. Poler

Dr. Brian Cooper

Dr. Jon Merkert

Importance of Study

Although fossil fuels provide valuable source of energy, the byproduct of burning of fossil fuels releases carbon dioxide gas which is the main contributing gas in climate change besides the emissions of other greenhouse gases that contribute in raising the average temperature of the Earth's climate system. Energy consumers and producers shifted to alternative energy sources, such as solar, tidal and wind energy, which have lower carbon emissions and do not have harmful consequences to the environment. However, the conventional energy is still the primary source of energy supply while the clean energy sources represent a small percent of energy consumption. This is due to lack of technical ways of storing energy from alternative sources to ensure the presence of supply when the sun sets, winds die and so on.

Batteries and capacitors are the common devices used to store energy. Batteries have high energy density, low power density and shorter life cycles while capacitors have a low energy density, high power density and longer life cycles. The energy storage can be improved by either improving the energy density of the capacitors or increasing the power density of batteries. If we develop new materials that have high surface area and provide higher energy density then it can be used as building materials for supercapacitors. Conventional double-layer capacitors store energy electrostatically through two separated electrode layers (electrical double-layer capacitance mechanism). The energy stored in the capacitor increases with the surface area of the separated electrodes. Since energy storage is directly proportional to the surface area of the capacitor layers, electrode material can be replaced with a substance that has a higher surface area; therefore, more energy can be stored, making those capacitors promising supercapacitors for future energy storage.

Nanoscale materials have smaller volumes and higher specific surface areas than bulk materials. In both energy storing devices (electrical double-layer capacitors and pseudo

capacitors), carbon nanotubes (CNTs) can be used as building materials of these capacitors; they have high electrical conductivity and high specific surface area (SSA) on which charges can be stored, making them viable materials in the production of these supercapacitors. Moreover, altering the surface of nanotubes and adding spacers could have a great impact on their functionality and make them good solutions for many environmental technical problems. However, CNTs tend to aggregate and reduce their SSA, making them less efficient as basic materials for many scientific applications. To prevent the self-assembly of CNTs and to increase the electron transfer and ion adsorption onto their surface and, therefore, increase the energy storage capabilities of these nanostructured carbon materials, molecular spacers were added.

Purpose Statement

We have studied single-walled carbon nanotubes (SWCNTs) for use as potential supercapacitor materials. Central to these applications are studies of the dispersion limit of SWCNTs in different solvents, and how various dinuclear coordination complexes interact with them. These complexes have high adsorption onto SWCNTs' surfaces and act as a "Molecular Spacer", which results in less aggregation. Keeping the nanomaterials from aggregating is required to maximize the ion accessible surface area (SSA). Higher dispersion stability due to the complementary interactions of the solvent and of the molecular spacers will be discussed. When the stability of SWCNTs-Molecular spacer assembly is enhanced, the capacity of the system improves. By increasing capacitance and preventing aggregation from molecular spacers, we hope to be able to use thin films as electrodes in supercapacitors.

Materials & Methodology

Dispersing solvent for the CNTs in this study, N,N-Dimethylformamide (DMF) (Fisher, Spectranalyzed). Single-walled carbon nanotubes investigated during this study include the SG 6,5 chirality and SG 7,6 chirality. SG 6,5 chiral tubes were produced by SWeNT® with >50% as (6,5)

chirality and tube diameters of 0.8 ± 0.1 nm. SG 7,6 chiral tubes were also produced by SWeNT® with >50% as (7,6) chirality and tube diameters of 0.93 ± 0.27 nm. To conduct dispersion stability measurements, molecular spacers were adsorbed on the surface of CNTs by adding different concentrations (0 μM – 1200 μM) of coagulants and left to incubate for 48 h. They were ultra-centrifuged at 100,000 g for 10 min to remove the aggregated tubes. Using UV-vis spectroscopy, the concentration of remaining CNTs in the supernatant were measured and normalized to the control pristine dispersion, and to conduct the Adsorption isotherm measurements, molecular spacers were adsorbed on the surface of CNTs by adding different concentrations of coagulants and left to incubate for 2 h. They were ultra-centrifuged at 10,0000 g for 1 h to remove the aggregated tubes. Using UV-vis spectroscopy, the concentrations of remaining CNTs in the supernatant were measured and normalized to the control pristine dispersion.

Expected to be Accomplished

Full characterization of different molecular coordination complexes with different size and chirality CNTs. Raman spectroscopy measurement will be conducted to both pristine and coordination complexes functionalized SWCNT-thin films formed on filter membranes. Electrochemical characteristics such as capacitance, energy storage, power dissipation, electrochemical impedance spectroscopy will be conducted with the complexes acting as molecular spacers between the SWCNTs in a condensed thin film. Also, Thin films of molecular spacers intercalated between different size and chirality CNTs will be studies by XRD, SEM AND TEM. Since the solvents might affect the stability of CNTs and how these tubes interact with the spacer. Dispersion stability of CNTs with two common dispersing non-aqueous solvents will be studied, *N*,*N*-dimethylformamide (DMF) and *N*-methyl-2-pyrrolidinone (NMP), and to insure the complete solubility of the spacers and to get higher dispersion stability different mixtures of the

solvents will be examined and the dispersion stability of CNTs will be measured. Dispersion characterization of hybrid nanoparticle assemblies, binding kinetics and adsorption isotherms will be conducted by light scattering technique monitoring particle size according to time and complex loading.