Introduction to Capacitor Sciences

Contents

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Introduction

Lithium ion batteries are the dominant energy storage device today, however, their inherent problems prohibit mass electrification. Capacitor Sciences created the materials to replace lithium ion batteries with high-energy density film capacitors. Capacitor Sciences' metadielectric materials increase the energy density, lifetime and safety of energy storage devices while reducing the cost of energy storage.

Capacitor Sciences is now scaling up the production of a series of metadielectric materials to produce and test product prototypes. The Company's molecular modeling and experimental results yield the performance required to produce capacitive energy storage devices with a capacity of 1 to 10+kWh/kg, four to forty times the energy density of commercially available lithium ion batteries.

Solving Energy Storage from First Principles

The ideal energy storage technology must address the following first principles:

1. Benign, low cost materials with high specific energies
2. Energy storage devices capable of over 10,000 cycles or 20 years of operation
3. Maintains its full energy storage capacity with no capacity degradation over its lifetime
4. Allows for safe and rapid charge and discharge
5. Scalable for electric vehicle, residential, commercial, industrial and utility applications

The Problem: High-Cost, Low Capacity & Flammable Batteries with Long Recharge Times

The dominant energy storage solution today is that of lithium ion batteries, however, they are fraught with problems. They are expensive. They have relatively low energy density. They lose capacity with each charge/discharge cycle. They can catch fire and explode. They require lithium and cobalt which are limited in supply. Furthermore, none of the proposed future battery chemistries are realistic solutions for low-cost, high energy density energy storage solutions. There is a fundamental need for safe, inexpensive, high capacity, rapidly rechargeable energy storage. Electrochemical batteries whether lithium ion, sodium ion, zinc-air or any other redox reaction based material system cannot provide that solution.

The Solution: Capacitive Energy Storage Devices Storing Energy in an Electric Field

Metadielectric materials that have polarizable cores and resistive envelopes can create high performance energy storage capacitors. In this material system energy is stored when an external electric field polarizes the electron cloud of polycyclic aromatic molecular cores. This stored energy is maintained within the structured crystalline film by insulation provided by the envelope of hydrocarbon tails. These composite metadielectric materials are designed to perform multiple functions that are not possible in inorganic crystalline materials, including self-assembly to form flexible crystalline films, polarizability to absorb energy and resistivity to store energy.

Industrial-Grade Capacitors for Energy Storage

Capacitor Sciences is developing a film capacitor that employs standard capacitor design and standard capacitor manufacturing techniques. The innovation that Capacitor Sciences brings to standard industrial capacitors is that of replacing the standard polypropylene dielectric film with the Company's polarizable and resistive metadielectric film. Similar to biaxially oriented polypropylene, Capacitor Sciences' dielectrophore materials are highly plastic and elastic, enabling them to withstand the high pressures that develop between oppositely charged electrodes. The electrodes, leads, potting and housing remain the same. Commercially available industrial grade capacitors have operational life-times of between 10,000 hours and 100,000 hours with minimal damage to the dielectric material and electrode systems. The Company's capacitive energy storage devices should achieve the same operational life-times and when translated into daily energy storage cycles (assuming 1 capacitor hour = 1 energy storage cycle) should far exceed the capacity-lifetime performance of lithium ion batteries. When manufactured, industrial-grade metadielectric capacitive energy storage devices will endure over 10,000 charge/discharge cycles without reducing the capacity of the metadielectric film resulting in a low Levelized Cost of Energy Storage per cycle.

Materials Originating from Oil for Global-Scale Energy Storage

The scale of production of energy storage materials required to store globally consumed electricity can be understood with the following analysis. Assuming an energy storage device with a specific energy of 1 kWh/kg one can determine the amount of material required to store 24 hours of globally consumed electricity. The EIA in its International Energy Outlook 2016 report estimates global electricity production to surpass 25,000 billion kWh in 2020 growing to over 35,000 billion kWh in 2040.

- 25,000 billion kWh/year divided by 365 days/year = 68 billion kWh/day
- 68 billion kWh/day divided by 1 kWh/kg = 68 billion kg of energy storage materials
- 68 billion kg/1000 kg/tonne = 68 million tonnes of energy storage materials
- 68 million tonnes / 10 years = 6.8 million tonnes per year of energy storage materials
- Rounding up yields 10 million tonnes per year of 1 kWh/kg energy storage materials

The scale of energy storage material production required for 24 hours of global electricity consumption can now be compared with the global production of commodity materials that could also be used for energy storage. Following are commodity materials and their respective annual production:

- Global electricity storage 1kWh/kg material requirement: 10 million tonnes per year
- Polyethylene: 80 million tonnes per year
- Polyethylene Terephthalate (PET): 30 million tonnes per year
- Polypropylene (PP): 1 million tonnes per year
- Lithium: 0.047 million tonnes per year (300 million tonnes lithium per year required)

In order to provide for global energy storage lithium production must increase by at almost 4 orders of magnitude to meet the required production demand. Polyethylene and polypropylene are produced in the quantities required to provide materials on the scale of 10 million tonnes per year needed to deploy global energy storage, however, an equivalent global manufacturing capacity will need to be developed. The only raw material able to support the required 10 million tonnes per year production capacity for global energy storage is oil. It is inexpensive, abundant and easily modified to produce high specific energy metadielectric materials at the scale required for global electricity storage.

Storing Energy

Today, in the US, energy is stored primarily in the strategic oil reserve (36 days of oil consumption), the gasoline we have in the tanks of the ~260 million cars registered in the US (350 miles per tank) and in the 40 pumped hydro facilities storing 22 GW of power generation capacity (2% of power generation for ~12 hours). The world has no meaningful energy storage capacity.

Demand for energy storage (rechargeable batteries) first increased with the introduction of mobile electronic devices (mobile phones, notebook computers, tablets and cameras). The second increase in demand for energy storage (rechargeable batteries, flywheels, …) resulted from the introduction of wind and solar PV generation in utility, industrial, commercial and residential markets. The third increase in demand for energy storage (rechargeable batteries) is a result of the introduction of electric vehicles (EVs) and the need to recharge their batteries without disrupting the electric grid. The fourth increase in demand for energy storage (rechargeable batteries) is arising from the economic and decarbonization benefits of distributed renewable energy resources and the market realization that electric motors will displace internal combustion engines (ICEs).

Tesla has started production of its Model 3 and has announced its electric Semi. Volvo announced its plans by 2019 to produce only EVs and hybrid vehicles. Daimler is partnering with BAIC in China to build a gigafactory to support the shift from ICEs to EVs. Volkswagen stated that 40 gigafactories will be needed by 2025 to supply the global EV industry. France and Germany announced that after 2040 sales of combustion engine based cars will be prohibited. The market trend is clear – there is a fundamental migration from internal combustion engines to electric motors driving the energy storage market. The charging of EVs also requires energy generation, distribution and storage infrastructure further increasing the demand for energy storage systems. Renewable energy requires a network of energy storage to accommodate the intermittency of wind and solar PV energy generation. In China over 30 million electric bicycles are produced and sold annually resulting in far more electric bicycles than cars.

The energy storage market faces an inflection point. The dominant energy storage solution today is that of lithium ion batteries, however, they are fraught with problems. They are expensive. They have relatively low energy density. They lose capacity with each charge/discharge cycle. They can catch fire and explode. They require lithium and cobalt which are limited in supply. Furthermore, none of the proposed future battery chemistries are realistic solutions for low-cost, high energy density energy storage solutions.

A new solution for energy storage is needed to realize the vision of global proliferation of EVs, supporting charging infrastructure and decarbonized energy generation. Capacitor Sciences has developed the technology to provide the global energy storage solution.

Capacitors and Batteries for Energy Storage

There are myriad schemes with which to store energy including pumping water from low lying reservoirs up to higher altitude reservoirs (pumped hydro), compressing air in tanks or caves (CAES), rapidly spinning heavy wheels (flywheel), pumping ionic liquids through a membrane (flow battery) and moving heavy weights up and down (gravitational potential energy storage). While creative, these energy storage schemes are construction projects occasionally suitable for utility-scale energy storage but are not deployable in electric vehicle, residential, commercial and industrial applications. The only viable energy storage technologies able to meet the energy storage needs (energy density, cost and application flexibility) are batteries and capacitors.

Lithium ion batteries are the dominant energy store today and there are plans to greatly expand their global production capacity. However, lithium ion batteries suffer from high levelized cost per cycle, capacity degradation and limited lithium and cobalt supplies. In addition, lithium dendrite growth causes anode-to-cathode short circuits resulting in fires and explosions.

Capacitors are the simplest passive electronic devices and have long been used for short duration energy storage for power applications. Film capacitors are inexpensive to produce, safe to operate and have none of the capacity degradation problems that plague batteries. Capacitor Sciences has developed the metadielectric materials technology to create capacitive energy storage devices for applications such as electric vehicles, charging stations, and residential, commercial, industrial and utility energy storage systems.

The Ideal Energy Storage Device

In contemporary electrical systems capacitors are used to deliver stored power (watts) and batteries are used to deliver stored energy (watt-hours). The ideal energy storage device should be able to deliver both stored power and stored energy.

Batteries are an electrochemical device storing energy in the chemical potential of a metallic oxide. While able to store energy at a relatively low energy density, these devices degrade during rapid charge and discharge. Therefore, batteries are not an appropriate device for delivering stored power but are the established standard for delivering stored energy.

The ideal energy storage device is one able to deliver power and to deliver energy without the need to differentiate between those tasks and without the degradation of its performance over the course of its use. Since the battery, by its nature, cannot become a power device the capacitor must then become an energy storage device.

Film capacitors are simple electrical energy storage devices comprised of a nonconductive, polarizable material (dielectric) between two metallic electrodes. The polarizability of the dielectric stores electrical energy while the insulative property of the dielectric prevents electrons from traveling from the negative electrode to the positive electrode retaining the stored energy. Biaxially oriented polypropylene is not polarizable to the degree necessary for high energy density storage devices.

To increase the energy density of a capacitor the polarizability of the dielectric must increase by orders of magnitude and the resistivity of dielectric material must be maintained. These two properties are not found in a single material but can be achieved by combining polarizable molecules with insulative molecules through the synthesis of organic materials.

The ideal energy storage device is then comprised of a metamaterial, a material not found in nature but one containing molecules that provide specialized functions of polarizability and resistivity, that self-assembles into a structured film. This structured film must withstand the pressure created by the attraction of the positive and negative electrodes and must maintain its crystalline order to hold the stored energy.

The ideal energy storage device is one in which only electrons move. There are no reduction-oxidation reactions. There are no mechanical moving parts. There are no changes in elevation.

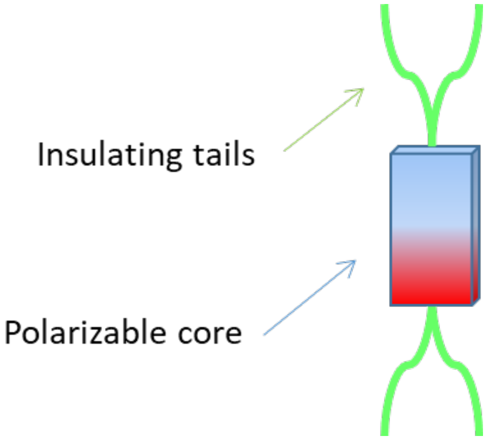
When charging the ideal energy storage device, electrons are deposited upon the negative electrode causing the electron cloud with the polarizable unit of the metadielectric material to shift away from the negative electrode creating an internal counter-field. The insulating unit of the metadielectric material prevents electrons from conducting to the positive electrode, maintaining the energy stored within the counter-field of the metadielectric polarizable unit. When discharging the ideal energy storage device, electrons are drawn from the negative electrode and the distorted electron cloud within the polarizable unit the metadielectric material returns to its zero-field state.

It is possible to create this ideal capacitive energy storage device. There is no limit to the degree of polarizability of dielectric materials. Most polarizable materials are semiconductors or conductors and require insulating molecules and an ordered structure to prevent charge leakage. Metadielectric capacitive energy storage devices are the embodiment of the ideal energy storage device.

Key Molecular Functions: Polarizability and Resistivity

Polarizability and Resistivity

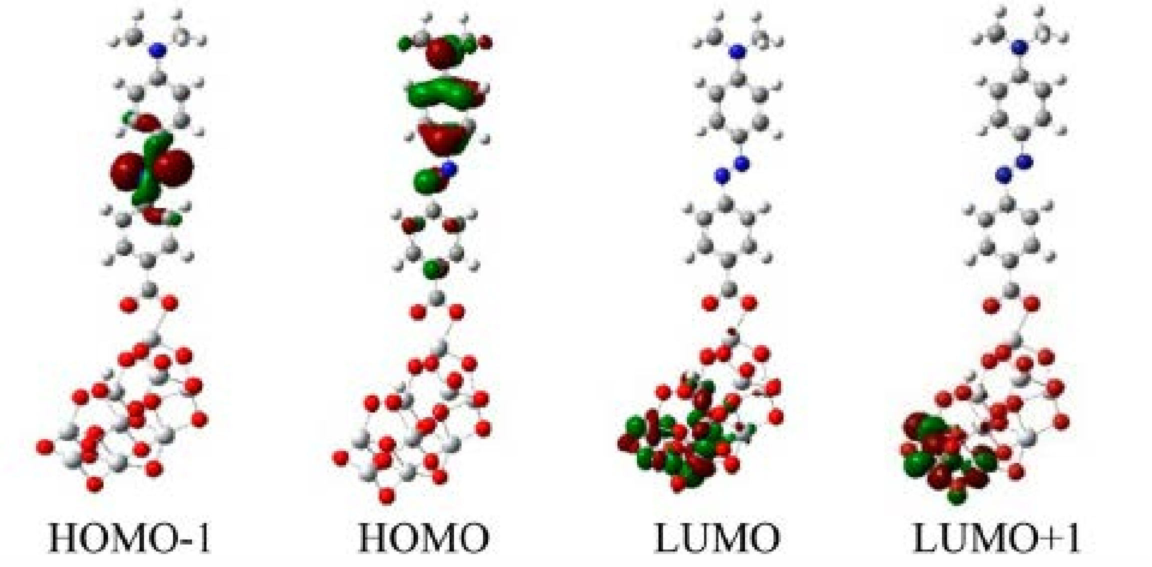
The two key functions of dielectrophores for energy storage are the polarizability of the carbon ring core (storing energy) and the resistivity of the carbon chain tails (holding energy). Energy is stored in the polarizable core and energy is maintained by the insulative tails of the metadielectric molecules.



Polarizability

Capacitor Sciences employs compounds with molecule cores comprised of carbon rings such as nonlinear optics inspired azo-dyes. The electron clouds of these core molecules absorb the energy from an external electric field (force) by promoting electrons from a lower energy level (Highest Occupied Molecular Orbit or HOMO) to a higher energy level (Lowest Unoccupied Molecular Orbit or LUMO) and distorting the electron cloud away from the negative electrode of the capacitor (distance). Work is defined as Force multiplied by Distance and in the case of capacitive energy storage is the result of the polarizability of the molecule and of the structured film. The more polarizable the core, the greater the energy density of the metadielectric material.

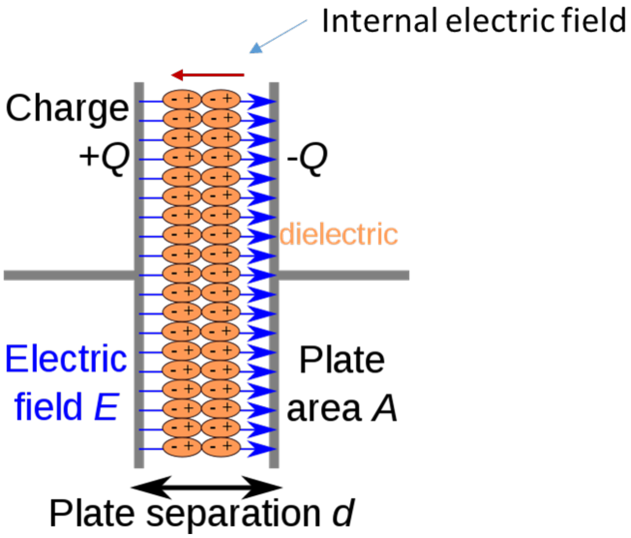
Upon excitation, the electron cloud shifts within the dielelectrophore. This shift in position within the molecular core is the Distance part of the energy absorption mechanism. The following diagrams depict the movement of electron density within azo-dye molecules as energy is absorbed promoting electrons from HOMO-1 to LUMO+1 energy states.



Azo-dye molecules depicting electron movement (Distance) from HOMO to LUMO states

Taken together, Force (electron cloud attraction to the positive charges of an atoms' protons) multiplied by Distance (electron cloud displacement from its zero-field state) yields Work (energy storage). This is the fundamental molecular mechanism behind Capacitor Sciences' dielectrophores' ability to absorb and store energy.

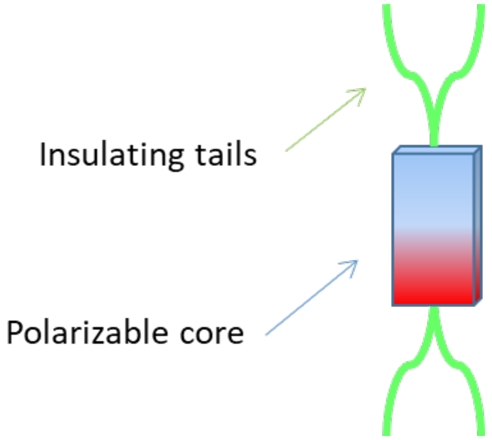
Displacement of electrons from their zero-field position produces an electric field opposite to the external applied electric field. The more loosely held the electron is in the molecular structure, the less energy required for its displacement and the more closely the external field is canceled by the internal field of electron displacement. Following is an illustration of the dielectrophore capacitor with the applied external electric field and the resulting internal electric counter-fields. As this is an electrostatic system the internal electric counter-field must be equal to the applied electric field.



Dielectrophore capacitor with applied electric field and resulting electric counter-fields

Resistivity

While the polarizable cores absorb energy from an external electric field, the insulative tails, comprised of hydrocarbon chains, insulate the cores and prevent electrons from traveling to adjacent molecular cores and eventually to the positive electrode. This insulative function provides the resistivity, or the ability for the metadielectric polarizable core to hold the energy absorbed by the external electric field.

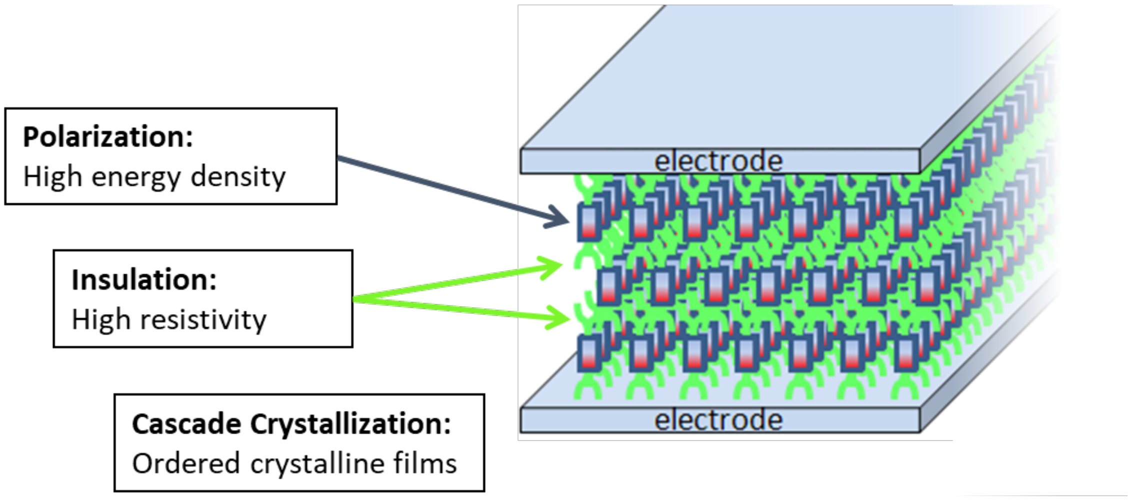


Polarizable dielectrophore cores and insulative tails

Key Film Function: Crystalline Structure for Polarizability and Resistivity

In order for the metadielectric materials to absorb and hold the energy absorbed from the external electric field a structured film must be produced that has continuous barriers to electron transfer. The design of the core and tail molecules enable a structured film to be produced by self-assembly. In the case of azo-dye cores the π-π interaction promotes core-to-core stacking perpendicular to the plane of the electrodes. In crystalline formation, the tails form a barrier structure that prevents electrons from transferring from one group of cores to another. In a structured crystalline film, the energy storage function of the cores and resistive function of the tails define the energy storage properties of bulk dielectrophore materials.

Following is a schematic diagram of a structured crystalline film between two electrodes displaying ordered and stacked cores with intertwined tails between core layers. The resistivity of the device depends upon structure of the film and, more specifically, upon composition of the insulating elements – in the simplest form comprised of alkyl tails. Electron conductivity in alkyl structures depends upon concentration of voids – empty sites that are formed in randomly aligned polymers during the process of solidification. By treating low density polyethylene with high pressure, the voids are closed, and the resistivity increases approximately two orders of magnitude. The same type of effect is observed in biaxially oriented polypropylene – introducing a higher order in the polypropylene film by stretching film in two directions industry increases resistivity of polypropylene by approximately two orders of magnitude.



Continuous layers of ordered insulating material prevent transport of electron in the structure and provide the same level of resistivity as bulk insulating material conventional in capacitors currently produced. It is significant that dielectrophores with 50-70% of polarizable semiconducting material within a structured insulating envelop of ordered layers of alkyl chains has the same level of resistivity as bulk insulating material.

Non-Linear Electro-Static Polarizability

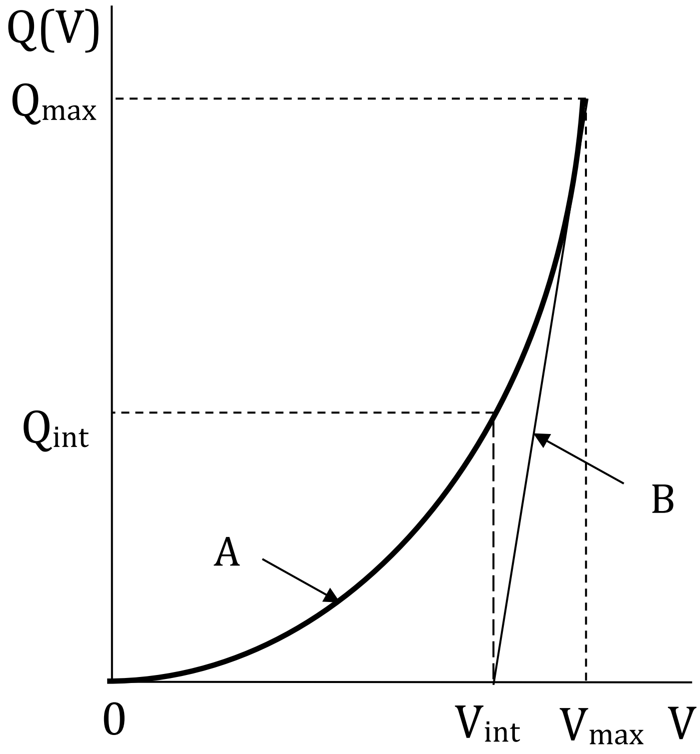
Capacitor Sciences employs polarizable cores inspired by the fields of non-linear optics (azo-dye oligomers) and polycycle conjugated heteroatomic aromatic compounds (rylene dyes) to which it attaches sp3 carbon insulating structures (aliphatic tails).

Both material systems exhibit nonlinear responses to excitation from light or from an external electric field. In nonlinear optics the azo-dye dielectrophore's index of refraction increases with increased applied voltage. This property was useful in steering a beam of light for optical switching. In capacitors the dielectrophore's polarizability increases with increased external electric field. As more electrons are applied to the negative electrode the counterfield within the dielectrophore increases nonlinearly. The relationship between specific energy [Wh/kg] and non-linear polarizability of the molecular core resulting from an external electric field is as follows:

Specific Energy [Wh/kg] is proportional to $\alpha E + \beta E^2 + \gamma E^3 + \dots$

The above Taylor series is a mathematical abstraction of the nonlinear effects of the interactions between the external electric field, the dielectrophore electron cloud and the dielectrophore protons. This approximation is useful only in that it focuses attention on the increased force required to displace subsequent electrons resulting in a near linear voltage regime as the dielectric material is charged and discharged.

The following plot illustrates the nonlinear effect of electron cloud polarization resulting from an external electric field. As applied charge (Q) increases the resulting voltage approaches a vertical asymptote defined by Vmax.



Nonlinear polarization - applied charge and resulting pseudo-constant voltage

This nonlinearity results from the increased energy required to distort successive molecular orbitals of dielectrophore electrons away from their protons and create a dipole. At the ground state the dielectrophore has an even distribution of electrons in various HOMO energy levels. As the dielectrophore encounters an external electric field, the most energetic HOMO-state electron orbitals are distorted away from their protons. As the distortion of HOMO-state electron orbitals continues, the remaining lower-energy HOMO electron orbitals require more energy to be distorted away from their protons. This successive increase in energy required to distort HOMO-state electron orbitals away from their protons is the mechanism that develops increasingly strong counter-fields and results in a nearly constant voltage as electrons are loaded upon the capacitor's anode.

In commercially available film capacitors the voltage varies significantly as the device discharges. In the dielectrophoric capacitor the voltage remains substantively constant as the device discharges. This nonlinearity significantly reduces the cost, weight, complexity and inefficiency of the power electronics required to deliver constant voltage from the discharging capacitor to the electric vehicle, home, business or utility employing the capacitive energy storage device. As the nonlinearity increases the resulting voltage, within a given charge density, closely approximates constant voltage perhaps eliminating the need for power electronics altogether.

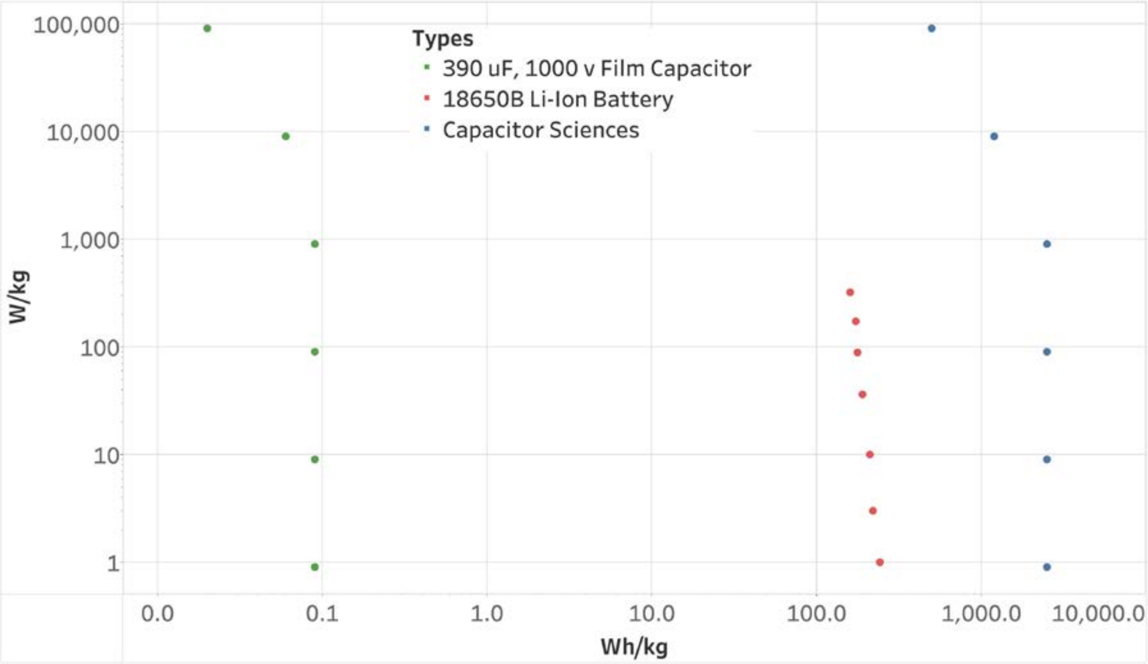
The variation in voltage is a function of applied charge to the 1/n degree where n = 4 or 5 for various classes of dielectrophore materials:

$$\Delta V = Q^{(1/n)}$$

Nonlinear expression of change in voltage with applied charge

The Ultimate Device Delivering Power and Storing Energy

Currently, capacitors have low energy density (– 3 Wh/kg) and high power density 100 kW/kg) suitable for power applications. Batteries have moderate energy density (250 Wh/kg) and low power density (300 – 500 W/kg) suitable for energy storage applications. The Ragone Chart was developed to visualize the relationship between specific power (W/kg) and specific energy (Wh/kg) for capacitors and energy storage systems. Below is a Ragone plot of commercially available film capacitors, lithium ion batteries and projected capacitive energy storage devices produced with Capacitor Sciences dielectrophores.



Ragone Plot for Capacitor Sciences, 18650 Li Ion Battery and Industrial Film Capacitor

The above Ragone Plot depicts the specific power vs specific energy profiles of a commercially available film capacitor (high power, low energy), of an 18650 lithium ion battery (low power, medium energy) and of a projected capacitive energy storage device manufactured with Capacitor Sciences dielectrophore materials (high power, high energy).

The ideal energy storage device is one able to deliver power and to deliver energy without the need to differentiate between those tasks and without the degradation of its performance over the course of its use. Since the battery, by its nature, cannot become a power device the capacitor should then become an energy storage device.