

Nano-scale Design of electrode materials for lithium rechargeable batteries

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Lithium rechargeable batteries have been widely used as key power sources for portable devices for the last couple of decades. Their high energy density and power have allowed the proliferation of ever more complex portable devices such as cellular phones, laptops and PDA's. For larger scale applications, such as batteries in plug-in hybrid electric vehicles (PHEV) or power tools, higher standards of the battery, especially in term of the rate (power) capability and energy density, are required. In PHEV, the materials in the rechargeable battery must be able to charge and discharge (power capability) with sufficient speed to take advantage of regenerative braking and give the desirable power to accelerate the car. The driving mileage of the electric car is simply a function of the energy density of the batteries. Since the successful launch of recent Ni-MH (Nickel Metal Hydride)-based HEVs (Hybrid Electric Vehicles) in the market, there has been intense demand for the high power-capable Li battery with higher energy density and reduced cost to make HEV vehicles more efficient and reduce emissions. However, current Li rechargeable battery technology has to improve significantly to meet the requirements for HEV applications not to mention PHEV.

In an effort to design and develop an advanced electrode material with high power and energy for Li rechargeable batteries, we approached to this in two different length scales - Atomic and Nano engineering of materials. In the atomic design of electrode materials, we have combined theoretical investigation using ab initio calculations with experimental realization. Based on fundamental understanding on Li diffusion, polaronic conduction, operating potential, electronic structure and atomic bonding nature of electrode materials by theoretical calculations, we could identify and define the problems of existing electrode materials, suggest possible strategy and experimentally improve the electrochemical property. This approach often leads to a design of completely new compounds with new crystal structures. In this seminar, I will talk about two examples of electrode material study under this approach; $\text{LiNi}_{0.5}\text{Mn}_{0.5}\text{O}_2$ based layered materials and olivine based multi-component systems. In the other scale of approach; nano engineering; the morphology of electrode materials are controlled in nano scales to explore new electrochemical properties arising from the limited length scales and nano scale electrode architecture. Power, energy and cycle stability are demonstrated to be sensitively affected by electrode architecture in nano scales. This part of story will be only given summarized in the talk.

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