Novel Cathode Materials for Lithium-ion Batteries

Lithium-ion batteries (LIBs) have become the most important energy storage devices and are widely applied on various fields in modern life. As a key component of a lithium-ion battery, the cathode material attracted considerable research attention. Up to now, various cathode materials for LIBs have been developed and exhibit good electrochemical performance, including lithium cobalt oxide ($LiCoO_2$), spinel material ($LiMn_2O_4$), polyanion material ($LiFePO_4$, $LiFeSO_4F$), silicate material (Li_2FeSiO_4). A selection of representative materials and corresponding crystal structures of those cathode materials are presented in Figure 1.

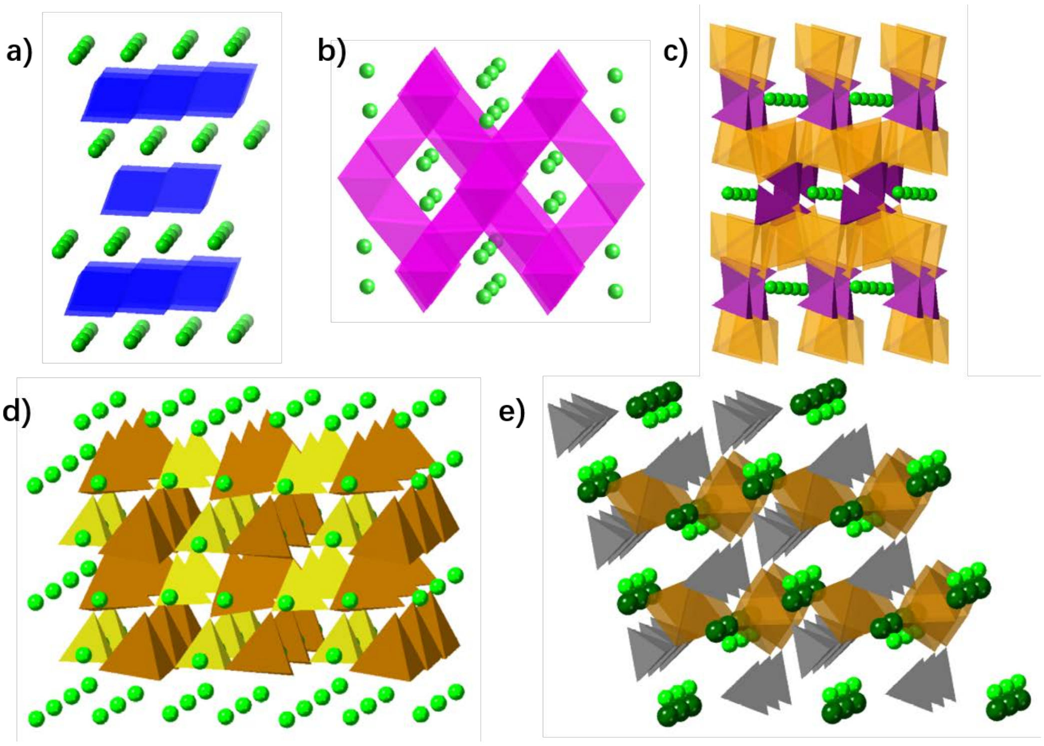

Figure 1. Representative crystal structures of cathode materials for lithium-ion batteries: (a) layered α-$LiCoO_2$; (b) cubic $LiMn_2O_4$ spinel; (c) olivine-structured $LiFePO_4$; (d) β_{II}-Li_2FeSiO_4; and (e) tavorite-type $LiFeSO_4F$. The light green spheres represent Li ions.

Although these inorganic cathode materials display good electrochemical performance and some of them have been applied in commercial LIBs, they still face some problems, such as low electronic conductivity. Carbon coating is regarded as the most efficient way to improve the conductivity and electrochemical performance of such inorganic cathode materials. Among various carbon materials, conducting polymers (CPs) gains more and more attention recently, due to the dual property of polymer's flexibility and conductor-like conductivity. Conducting polymers cannot only be composited with conventional inorganic materials to form hybrid cathodes, but also be directly applied as electrodes of Li-ion batteries due to the conversion redox mechanism. A verity of conductive polymers have been developed for the applications of electrodes, including polyacetylene (PA), polyaniline (PANI), polypyrrole (PPy), polythiophene (PTh), poly(para-phenylene) (PPP), poly(para-phenylene vinylene) (PPV), polyfuran (PF), and poly(3,4-ethlenedioxythiophene) (PEDOT). The molecular structures of these typical CPs are displayed Figure 2.

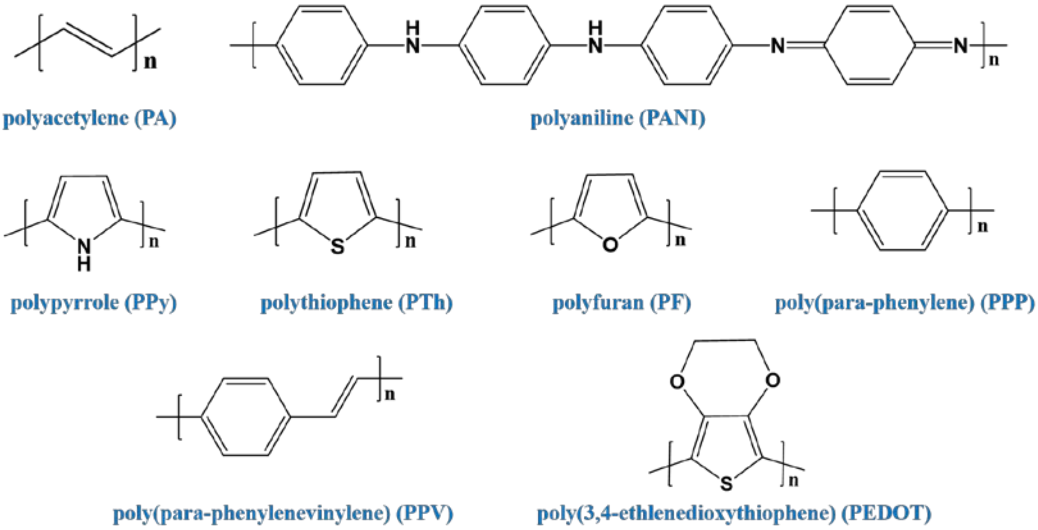

Figure 2. Molecular structures of typical conducting polymers applied in cathodes of lithium-ion batteries.

In order to optimize inorganic/organic (CPs) cathode materials, it is necessary to deeply understand the relationship between structural changes of the cathodes and the electrochemical performance of the batteries. This understanding can be obtained by in-situ and in-operando characterization techniques, which provide information of the structure evolution during electrochemical processes. Grazing incidence X-ray scattering (GIXS) techniques are very powerful methods to probe the morphology evolution of electrode materials during charge/discharge processes [1,2]. With grazing incidence wide angle X-ray scattering (GIWAXS), the crystal structure and orientation of the conducting polymer can be investigated. These properties of the conducting polymer can affect its conductivity as well as the final electrochemical performance of the battery with such hybrid cathodes. In addition, the structure changes from nano-scale to submicron-scale inside the cathode materials can be probed by grazing incidence small angle X-ray scattering (GISAXS). Based on these in operando investigations on the morphologic and structural changes of the inorganic/organic (CPs) cathode materials, better electrochemical performance of batteries will be developed.

Featured publications:

[1] P. Müller-Buschbaum: Structure determination in the thin film geometry using grazing incidence small angle scattering; *“Polymer Surfaces and Interfaces: Characterization, Modification and Applications”,* edt. M. Stamm, Springer Berlin, ISBN-13: 978-3-540-73864-0, 17-46 (2008).

[2] P. Müller-Buschbaum: A basic introduction to grazing incidence small angle X-ray scattering; special issue of L*ecture Notes in Physics on "Applications of Synchrotron Light to Noncrystalline Diffraction in Materials and Life Sciences"*, Vol. 776, edt. Ezquerra, T.A.; Garcia-Gutierrez, M.; Nogales, A.; Gomez, M., Springer Berlin, ISBN: 978-3-540-95967-0, 61-90 (2009).