Keynote Lecture

KN15

Impact of Crystallography on Design of Cathode Materials for Li-ion Batteries

E. Antipov[1], N. Khasanova
[1]*Lomonosov Moscow State University, Department of Chemistry, Moscow, Russia*

Ninety percent of the energy produced today come from fossil fuels, making dramatically negative impact on our future due to rapid consumption of these energy sources, ecological damage and climate change. This justifies development of the renewable energy sources and concurrently efficient large storage devices capable to replace fossil fuels. Li-ion batteries have originally been developed for portable electronic devices, but nowadays new application niches are envisaged in electric vehicles and stationary energy storages. However, to satisfy the needs of these rapidly growing applications, Li-ion batteries require further significant improvement of their properties: capacity and power, cyclability, safety and cost. Cathode is the key part of the Li-ion batteries largely determining their performance. Severe requirements are imposed on a cathode material, which should provide fast reversible intercalation of Li-ions at redox potential close to the upper boundary of electrolyte stability window, possess relatively low molecular weight and exhibit small volume variation upon changing Li-concentration. First generation of the cathode materials for the Li-ion batteries based on the spinel (LiM2O4, M – transition metal) or rock-salt derivatives (LiMO2) has already been widely commercialised. However, the potential to further improve the performance of these materials is almost exhausted. The compounds, containing lithium and transition metal cations together with different polyanions (XmOn)p- (X=B, P, S, Si), are now considered as the most promising cathode materials for the next generation of the Li-ion batteries. Covalently-bonded structural frameworks in these compounds offer long-term structural stability, which is essential for good cyclability and safety. Further advantages are expected from combining different anions (such as (XO4)p- and F-) in the anion sublattice, with the hope to enhance the specific energy and power of these materials. Various fluoride-phosphates and fluoride-sulphates have been recently discovered, and some of them exhibit attractive electrochemical performance. An overview of the research on the cathode materials for the Li-ion batteries will be presented with special emphasis on crystallography as a guide towards improved properties important for practical applications.

Keywords: Li-ion batteries, crystal structure, cathode materials