

Case ID:M12-155P

Published: 10/3/2012

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Transition metal hydroxy-anion electrode materials for lithium-ion battery cathodes

The lithium battery industry is undergoing rapid expansion, now representing the largest segment of the portable battery industry and dominating the computer, cell phone, and camera power source industry. High capacity and high rate lithium-ion batteries (LIB) with low cost and improved safety characteristics constitute a major requirement for electric vehicles, portable electronics, and other energy storage applications. Year-to-year electrochemical performance improvements in LIBs are typically limited to 3-4%, with a major bottleneck being the lack of appropriate materials to satisfy the energy and power density requirements. From a technology perspective, the key bottleneck is mainly on the cathode side. Despite more than 30 years of research, and expansion from the initial studies of layered sulfides to oxides and now polyanion materials, current cathodes have practical capacities of only 150-180 mAh/g. While nanostructuring of existing cathodes has been found to lead to improvements in usable charge capacity and result in higher rate performance, the theoretical capacities of existing materials is still too low. There is a need for the discovery of new materials that can participate in higher capacity charge storage reactions.

Researchers at Arizona State University have developed the use of transition metal hydroxyl anion materials (such as hydroxysulfates and hydroxyphosphates) as cathode materials for Lithium ion batteries. These materials fall into a class of materials known as polyanions. Polyanion materials have shown promising electrochemical performance as cathodes in lithium ion batteries in terms of their capacity (100-170 mAh/g), reaction potential, cyclability, and safety. However, these materials still suffer from low intrinsic charge storage capacities and poor electronic conductivity due to their intrinsic bonding and structure. A family of materials based on transition metal hydroxysulfate or hydroxyphosphate naturally occurring minerals offers the possibility for improved performance as cathode materials due to the following characteristics: (1) open framework or layered structures that can facilitate fast Li⁺ insertion, (2) beneficial bonding characteristics such as edge sharing MO₆ octahedra for good electronic conductivity and improved rate performance, (3) flexibility in alkali and transition metal cation incorporation as observed in nature, which can allow for the design of solidsolutions to enhance structural stability, capacity, and reaction potentials, and (4) possibility for multielectron redox reactions due to the incorporation of greater than 1 transition metal per formula unit, which can result in capacities greater than 200 mAh/g.

Related publications:

[Electrochemical Properties of Nanostructured Copper Hydroxysulfate Mineral Brochantite upon Reaction with Lithium](#)

Synthesis of Jarosite and Vanadium Jarosite Analogues Using Microwave Hydrothermal Reaction and Evaluation of Composition-Dependent Electrochemical Properties

Potential Applications:

- Lithium Ion Batteries
- Hybrid Electric Vehicles
- Electric Vehicles
- Portable Electric Devices
- Renewable Energy Storage

Benefits and Advantages:

- Improved charge capacity at the cathode
- Tailorability of designs through chemistry to optimize performance
- Open framework design to facilitate Lithium ion insertions