Copper-Based Metal-Organic Frameworks as Cathode Material for Rechargeable Batteries

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Over the last years, metal-organic frameworks (MOFs) have emerged as a versatile and promising class of materials for various aspects in energy storage systems.[1] These materials are characterized by a crystalline structure composed of metal ions or inorganic clusters (often referred as "SBU": "secondary building unit") coordinated to multivalent organic molecules, also called "linker". Due to the inorganic/organic hybrid structure, MOFs exhibit well-dispersed metal centers separated by organic linkers, which can be equipped with a variety of functional groups. MOFs have normally a microporous structure with well-defined pore sizes tailorable by the length of the incorporated linker molecules. The hybrid composition of MOFs leads often to flexible crystal structures that withstand the insertion and removal of guest molecules (*e.g.* solvent molecules) or ions (cations or anions) due to reversible structural changes. As multivalent metal ions in the SBU and also organic linker molecules can offer redox-active sites, MOFs gain increasingly attention in electrocatalysis and battery applications.[2] MOFs are particularly interesting for anion insertion on the positive electrode since well-defined pore sizes and redox-activity facilitate a reversible anion exchange in the dual-ion battery concept.[3] Inherent to most metal-organic frameworks is a low electronic conductivity due various aspects, but in general due to the organic parts of the structure.[4]

In the present work, we have synthesized a copper-based MOF with a radical anionic linker showing a relatively high electronic conductivity despite the inorganic/organic hybrid structure. The Cu-MOF was successfully applied as an anion storage material on the positive electrode in a lithium metal cell. Constant current cycling studies reveal a high specific capacity and a high capacity retention for more than 100 cycles. Using X-ray photoelectron spectroscopy (XPS) and *in-situ* X-ray diffraction (XRD) techniques, the redox reaction behavior of the copper metal ion and the structural properties of the Cu-MOF were investigated during charge/discharge operation. MOF-based composite electrodes were prepared *via* an electrode paste coating process, which makes the MOF readily adaptable for an up-scaled battery electrode production.

References:

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