Lithium Copper Phosphates as High Energy Density Li-ion Cathode Materials

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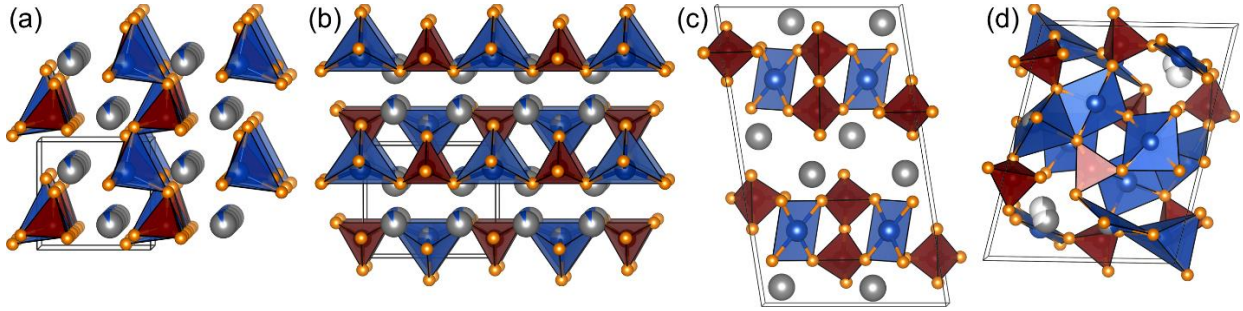

Reported structures of (a) $Li_{2.05}Cu_{0.95}PO_4$ projected nearly down the a-axis and (b) the structure projected nearly down the c-axis.[1] The structures of (c) $Li_2CuP_2O_7$ projected nearly down the b-axis. (d) The structure of $Li_2Cu_5(PO_4)_4$ projected nearly down the a-axis.

Three compositions of lithium copper phosphates: Li_2CuPO_4, $Li_2Cu_5(PO_4)_4$, and $Li_2CuP_2O_7$ have been studied as high voltage cathode materials for Li-ion batteries, following computational predictions of high operating voltages. An assisted-microwave preparation of Li_2CuPO_4, which is otherwise difficult to prepare in nearly-pure form, has been developed. The electrochemical performance of all three compounds have been investigated. The cyclability of these materials is found to be poor due to structural changes, irreversible reduction to metallic copper even at potentials as high as 2.5 V, and the possibility of dissolution into the electrolyte. Some general understanding in regard to the use of Cu compounds in redox electrodes is presented.

This work and the Materials Research Laboratory are supported by the National Science Foundation through DMR-1720256. Support for this work from BASF through the California Research Alliance (CARA).

References:

1. K. Snyder, B. Raguz, W. Hoffbauer, R. Glaum, H. Ehrenberg, and M. Herklotz. Lithium Copper(I) Orthophosphates $Li_{3-x}Cu_xPO_4$: Synthesis, Crystal Structures, and Electrochemical Properties, *Z. Anorg. Allg. Chem.* **640** (2014) 944–51.