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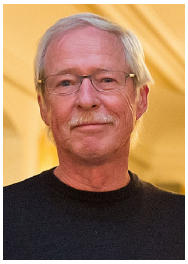
BATTERIES & SUPERCAPS
Cover Profile

Elucidation of the Sodium–Copper Extrusion Mechanism in $CuCrS_2$: A High Capacity, Long-Life Anode Material for Sodium-Ion Batteries





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The front cover artwork is provided by the group of Prof. Bensch at the inorganic chemistry department of Christian-Albrechts-University Kiel (Germany). The image illustrates the copper – sodium extrusion mechanism in $CuCrS_2$ during the first step of sodium uptake. Additionally, the results of ex-situ X-ray diffraction measurements and pair distribution function measurements are displayed. Read the full text of the article at 10.1002/batt.201800039.

What aspects of this project do you find most exciting?

While working on this project, it became clear how important it is to investigate the results more closely. Because the sodium – copper extrusion mechanism is well known, we expected a simple phase transition of $CuCrS_2$ to $NaCrS_2$ and Cu during the early stage of sodium uptake. A first comparison of the X-ray data seemed to confirm this assumption. But a closer look, and thorough Rietveld refinements of the ex-situ XRD data unveiled the presence of about 15% Cu^+ still occupying the tetrahedral position, resulting in a non-stoichiometric compound with the composition $Na_{0.70}Cu_{0.15}CrS_2$ and 15% of cation vacancies present in the structure. This shows that things are not always as simple as they look at first glance and scientists should keep this in mind more often.

What was the biggest surprise?

During the early stage of the first discharge of $CuCrS_2$, $Na_{0.7}Cu_{0.15}CrS_2$ and Cu nanoparticles are formed. To evaluate if these Cu particles have a beneficial impact on the electrode performance, we compared this material with $NaCrS_2$. Surprisingly, the positive effects in terms of rate capability and capacity retention of the nanoscopic Cu was much more pronounced than expected. The capacity of all $NaCrS_2$-cells quickly faded and was less than 100 mAh g^{-1} after 50 cycles, even at low current rates, while the $CuCrS_2$ electrodes still achieved about 420 mAh g^{-1} after more than 200 cycles.

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