## SnS<sub>2</sub> and C-SnS<sub>2</sub>/Si anode active materials for Li ion batteries

Akzhan Bekzhanov<sup>1, 2</sup>, Irshad Mohammad<sup>1</sup>, Freddy Kleitz<sup>2</sup>, Damian Cupid<sup>1,</sup> <sup>1</sup>AIT Austrian Institute of Technology GmbH <sup>2</sup>University of Vienna, Department of Functional Materials and Catalysis email: akzhan.bekzhanov@ait.ac.at

Tin-based chalcogenides such as  $SnS_2$  have been investigated as potential anode active materials for Liion batteries due to their high theoretical reversible capacities (e.g., 644 mAh g<sup>-1</sup> for  $SnS_2$ ). These high capacities are associated with the reversible alloying of Sn with Li after the conversion reaction of  $SnS_2$  to Sn and Li<sub>2</sub>S. The hydrothermal method is known to be a facile, sustainable procedure to synthesize electroactive materials without utilizing surface active agents and other additives. However, the influence of precursor ratios on crystal structure, particle morphology and electrochemical performance is usually not carefully explored in literature. Therefore, in present work,  $SnS_2$  was synthesized using different ratios of tin chloride and thioacetamide to investigate the structure-performance-property relationships of  $SnS_2$  anode active materials.

The synthesized  $SnS_2$  powders exhibited varied degrees of crystallinity and plane orientations depending on precursor ratio, as observed by Rietveld refinement of the measured X-ray diffraction (XRD) patterns. Specifically, increasing the molar ratio of S to Sn in solution yielded in more crystalline  $SnS_2$  products with intensified crystal plane orientations. During electrochemical analysis of the electrodes, which were prepared by water-based processing, a self-healing property could be identified, where the highly layered crystals showed reversibility of the conversion reaction of Sn and Li<sub>2</sub>S back to SnS<sub>2</sub>.

Also, we synthesized C-SnS<sub>2</sub>/Si composite anode material with a high energy density and excellent cycle stability via solid state method. The structure of C-SnS<sub>2</sub>/Si composite composite material is sandwiched like, where active materials are integrated into conductive porous polymer matrix. Using the structural advantages of composite material, the lithium storage mechanism of tin disulfide and silicon materials have been improved from three aspects: alleviating the volume expansion effect, improving the stability of the solid electrolyte interface (SEI), and enhancing the electrical conductivity. The material exhibits good performance when applied to lithium-ion battery anodes. At the current density of 0.1 Ah g-1, the specific discharge capacity of the electrode material is maintained at 510 mAh g-1 after 200 cycles for C-SnS<sub>2</sub>/Si material and 720 mAh g-1 after 100 cycles for C-SnS<sub>2</sub> composite anode material.

Keywords: tin disulfide anode; composite; carbon coating; matrix; silicon anode; solid state; synthesis

## Acknowledgement

This research work is funded by Project "RESTINA", where the main goal is to deliver "generation 3b cells for battery electric vehicles (BEVs)". Funding agent

M-ERA.NET has defined 6 quantified priorities, both in terms of their objectives and their budgetary impact: 1) support basic research in all scientific fields, 2) intensify the strategic research, 3) amplify the international dimension, 4) develop interdisciplinary research, 5) encourage "risky" projects and 6) establish equipment and infrastructure at the service of fundamental research and innovation.