

## MM 3: Materials for Energy Storage and Conversion

## New Battery Materials

Time: Monday 10:15–11:30

Location: H44

MM 3.1 Mon 10:15 H44

**Li3OCl thin film as a solid state electrolyte** — •KUN ZHANG, EFI HADJIXENOPHONTOS, YUG JOSHI, and GUIDO SCHMITZ — Chair of Materials Physics, Institute of Materials Science, University of Stuttgart, Heisenberg Straße 3, 705969 GERMANY

In comparison with conventional batteries, solid state batteries offer safety and higher energy density. In this work, Li-rich Li3OCl is studied as a potential solid-state electrolyte in Li-Ion batteries. Thin Li3OCl films (50–200 nm) are deposited by applying a composite target (Li2CO3+LiCl) via Ion Beam Sputtering. The composition of the films is investigated by XRD and XPS, and the thickness is evaluated by FIB cross-sections. The ionic and the electrical conductivity are determined using Pt/Li3OCl/Pt structure by Electrochemical Impedance Spectroscopy and  $\sim 10^{-7}$  S/cm and  $\sim 10^{-11}$  S/cm are achieved respectively at 25 °C. Furthermore, the activation energy of Li3OCl is derived from the measured ionic conductivity from 25 °C up to 140 °C and is equal to 0.57 eV.

MM 3.2 Mon 10:30 H44

**Controlling oxygen defects in Li4Ti5O12 (LTO)** — •C. GROSU<sup>1,2</sup>, P. JAKES<sup>1</sup>, T. GIGL<sup>2</sup>, C. HUGENSCHMIDT<sup>2</sup>, D. HAERING<sup>2</sup>, J. GRANWEHR<sup>1</sup>, R.A. EICHEL<sup>1</sup>, K. REUTER<sup>2</sup>, and C. SCHEURER<sup>2</sup> — <sup>1</sup>IEK-9, FZ Jülich — <sup>2</sup>TU München

Spinel Li4Ti5O12 (LTO) is an interesting anode material for next-generation all solid state Li-ion batteries (ASSB). Its "zero strain" charge/discharge behavior promises high safety and long cycling lifetimes. Yet, pristine, white LTO possesses poor ionic and electronic conductivity. The latter can be increased by tailoring the sintering protocol to produce oxygen vacancies, resulting in a performing, blue LTO material. Hitherto, the detailed structure and distribution of the vacancies is not known. Producing a controlled gradient of vacancies will help understanding, first what the fundamental impact on the conductivity is and later optimizing the design of the material itself. We will discuss a controlled procedure to introduce oxygen vacancies, creating a gradient of defects from the surface to bulk. In a combined experimental and theoretical approach, the resulting disordered, defect-rich LTO structures are analyzed and theoretical defect models compared to the results of depth-resolved positron coincidence Doppler broadening spectroscopy (CDBS) measured at the Garching positron source NEPOMUC.

MM 3.3 Mon 10:45 H44

**Weberite-type sodium metal fluorides - promising cathode materials for sodium ion batteries** — •HOLGER EUCHNER<sup>1</sup>, ANJI REDDY<sup>1</sup>, OLIVER CLEMENS<sup>2</sup>, and GROSS AXEL<sup>1,3</sup> — <sup>1</sup>Helmholtz Institute for Electrochemical Energy Storage, Ulm, Germany — <sup>2</sup>Materials Design by Synthesis, Technical University Darmstadt, Darmstadt, Germany — <sup>3</sup>Institute of Theoretical Chemistry, Ulm University, Ulm, Germany

Among alternative battery technologies suggested for substituting the state of the art lithium-ion batteries (LIBs) Na ion batteries (NIBs) are one of the most promising candidates. However, due to the lower operating potential of the cathode material in current NIBs their specific energy is significantly lower than in LIBs. To compete with the high energy density of LIBs, high voltage cathode materials are required for NIBs. Here, we report a computational investigation of weberite-type

sodium metal fluorides (Na2MM'F7), a new class of so far unexplored high voltage and high energy density materials. A series of known and hypothetical compounds with weberite-type structure are investigated and their potential as cathode materials for NIBs is evaluated. Weberite-type Na2MM'F7 shows quasi-three-dimensional Na diffusion with surprisingly low activation barriers. The high energy density combined with low barriers for Na diffusion makes Na2MM'F7 type compounds promising candidates for cathode materials in NIBs.

MM 3.4 Mon 11:00 H44

**Highly nitrogen doped carbon nanofibers with superior rate capability and cyclability for potassium ion batteries** — •CHENGLIN ZHANG, YANG XU, LONG LIU, and YONG LEI — Institute für Physics & IMN MacroNano (ZIK), Technische Universität Ilmenau, Ilmenau 98693, Germany

Potassium-ion batteries are a promising alternative to lithium-ion batteries. However, it is challenging to achieve fast charging/discharging and long cycle life with the current electrode materials because of the sluggish potassium ion kinetics. Here, we report a soft carbon anode, namely highly nitrogen-doped carbon nanofibers, with superior rate capability and cyclability. Quantitative analysis and theoretical simulations were employed to interpret the benefits of nitrogen doping and demonstrate the advantage of the pyrrolic and pyridinic N dopants over the quaternary N dopant. Surface-dominated K-storage is verified by quantitative kinetics analysis and theoretical investigation.[1] Considering the cost-effectiveness and material sustainability, our work may shed some light on searching for K-storage materials with high performance.

[1] Yang Xu; Chenglin Zhang; Min Zhou; Qun Fu; Chengxi Zhao; Minghong Wu\* and Yong Lei\*[J] Nature Commun. (2018) 9:1720.

MM 3.5 Mon 11:15 H44

**2D/3D Organo-metal Hybrid Perovskite Photobatteries** — •ANGUS MATHIESON, FELIX DESCHLER, and MICHAEL DEVOLDER — University of Cambridge, Cambridge, United Kingdom

Increases in the global energy demand necessitate the development of new approaches to energy conversion and storage. In particular, the utilisation of solar energy could provide a basis of evolving technologies capable of meeting modern demands.

By combining the photovoltaic and newfound electrochemical properties of organo-metal hybrid perovskite materials in a single device, a novel photobattery technology is proposed. Utilising the photovoltaic performance of bulk 3D perovskite materials in combination with the intercalation and conversion mechanisms available to Lithium ion species of layered 2D perovskite materials, a device with the ability both to convert light to electrochemical energy and store it is discussed. The motivation for such a device will be demonstrated, with its inherent impact in areas such as off-grid energy solutions and the internet of things. The fabrication techniques are described and characterisation techniques common to both photovoltaic and electrochemical disciplines, with their recent results are discussed. The current understanding of the charge carrier dynamics and device structure under electrochemical cycling are discussed in depth followed by recent developments in device performance and characterisation. Given the potential commercial applicability of the device, ideas to enhance the device performance whilst reducing fabrication cost and increasing scale are used in conclusion.