

AKE 2: Processes and Materials for Energy Technologies

Time: Tuesday 9:30–11:30

Location: TC 006

Invited Talk

AKE 2.1 Tue 9:30 TC 006

Concepts for combining concentrating solar mirrors with PV modules — ●MORITZ RUHWEDEL^{1,2}, KAI GEHRKE³, ECKHARD LÜPFERT¹, FLORIAN SUTTER¹, PETER HELLER¹, and ROBERT PITZ-PAAL^{1,2} — ¹DLR (German Aerospace Center) Institute of Solar Research, Linder Höhe, 51147 Köln, Germany — ²RWTH Aachen University, Chair of Solar Technology, Linder Höhe, 51147 Köln, Germany — ³DLR (German Aerospace Center) Institute of Networked Energy Systems, Carl-von-Ossietzky-Str. 15, 26129 Oldenburg, Germany

Concentrating solar thermal (CST) technologies produce renewable, sustainable heat at elevated temperature. In this work four concepts are compared to integrate photovoltaic cells into CST heliostats and at tower receivers to increase efficiency and decrease cost of the systems. Based on previous research, parameters are derived which describe energy production and investment cost of the concepts. It is found that the integrated concepts can increase the total annual energy production of a concentrating solar power plant by 23% to 40%, justifying investment cost increase compared to the conventional configurations. According to this the concepts utilizing a spectrally selective mirror on top of PV cells to replace the concentrating mirrors are expected to be economically feasible. The concentrating PV concept produces electricity at lower cost than separate stand-alone PV if the spillage radiation flux around the receiver of CST tower plants is higher than around 350 kW/m².

AKE 2.2 Tue 10:00 TC 006

Novel approach of advanced characterization, dedicated synthesis and theoretical modelling on commercially relevant Fischer-Tropsch catalysts for production of sustainable fuels & chemicals: Bridging industry and academia — ●ANNA ZIMINA^{1,4}, RABIA ELBUGA-ILICA¹, DAN ZHAO¹, CHERIE HSU¹, ERISA SARACI¹, MORITZ WOLF¹, FELIX STUDDT¹, MICHAEL CLEAYS², DENZIL MOODLEY³, and JAN-DIERK GRUNWALDT^{1,4} — ¹IKFT-KIT / Eggenstein-Leopoldshafen / Germany — ²University of Cape Town / South Africa — ³Sasol South Africa / South Africa — ⁴ITCP-KIT / Karlsruhe / Germany

Power-to-liquid processes can be considered the key for renewable electricity-based liquid fuel generation. Various olefins can be synthesized via Fischer-Tropsch synthesis. The CARE-O-SENE consortium that connects German and South African partners is driven to accelerate the development of cobalt-based FT catalysts for green and efficient production of sustainable aviation fuel. For efficient development, systematic characterization of Co-based catalysts, especially in-situ and operando is essential to derive structure-activity relationships in reliable manner. X-ray absorption spectroscopy, X-ray diffraction, magnetometry and Raman spectroscopy are a highly promising tool as structural changes of active species, support and adsorbents can be observed in heterogeneous catalysts at work. Advanced studies of commercially relevant materials for FTS and model structures to mimic the atomic structure of active cobalt, promoter and support were performed and combined with theoretical modelling.

AKE 2.3 Tue 10:15 TC 006

first principle exploration of twisted hBN-NbSe₂ hetero-structure and application as an electrode for li-ion battery — ●SHUBHAM SAHOO and SOUMYA JYOTI RAY — indian institute of technology patna, bihta, india, 801106

In this work, we have designed a van der Waals hetero-structure made of conducting 2D NbSe₂ -layer and insulating hexagonal boron nitride (h-BN) and applied interlayer twist at different twist angles for potential application as an electrode in Li-ion battery. The hetero-structure offers a metallic character which makes the insulating h-BN capable of battery application. The adsorption site changes for different twist angles. For the twist angle of 5.21° and 54.79°, the H-site is the most favorable adsorption site but for all other twist angles, T-site stays the most favorable adsorption site. When the angle between surfaces is 19.11°, the hetero-structure shows better stability as compared to all other configurations in different twist angles. The adsorption energy gets enhanced compared to the individual mono-layers indicating better intercalation. At a twist angle of 19.11°, our structure is showing a minimum diffusion barrier of 0.6 eV whereas at all other twist angles, it shows nearly 0.9 eV barrier. The open circuit voltage is found to be

0.62 Volt. The structure is showing a specific capacity of 185 mAh⁻¹ gm⁻¹.

15 min. break

AKE 2.4 Tue 10:45 TC 006

Mn-substituted V₂C MXene as anode materials for Li-Ion batteries — ●TOBIAS KÖNIG¹, PENG GUO^{1,2}, TOM WICKENHÄUSER¹, LENNART SINGER¹, PETER COMBA², and RÜDIGER KLINGELER¹ — ¹Kirchhoff Institut für Physik, Universität Heidelberg, Im Neuenheimer Feld 227, D-69120 Heidelberg, Germany — ²Anorganisch Chemisches Institut, Universität Heidelberg, Im Neuenheimer Feld 270, D-69120 Heidelberg, Germany

The recently found class of layered materials, MXenes, has attracted attention as potential anode materials in lithium-ion batteries due to their high theoretical capacity as well as their long cycling stability. We report on the effect of a Mn-substitution in V₂C MXenes, i.e. VMnC, synthesised by different etching processes. The distinct peaks in cyclic voltammetry measurements of VMnC suggest that Mn-ions offer extra redox-active centers yielding an increase of the specific capacity compared to V₂C. Galvanostatic cycling with potential limitation studies show significantly larger reversible capacities of 370 mAh/g in VMnC, at a current of 100 mA/g, which exceeds 256 mAh/g observed in V₂C by more than 40%. Additional investigations show the impact of different etching solvents applied during the synthesis process of the MXenes. In contrast to the abovementioned performance of VMnC synthesized using HCl+LiF as an etching solvent, the specific capacity amounts to only 260 mAh/g when using HCl+NaF. We discuss this result with respect to the interlayer distances and sample morphology. Overall, Mn-substitution strongly affects and improves the electrochemical performance of V₂C MXenes.

AKE 2.5 Tue 11:00 TC 006

Elucidating the electrochemical reaction mechanism of lithium-rich antiperovskite cathodes for lithium-ion batteries as exemplified by (Li₂Fe)SeO — ●LENNART SINGER¹, M.A.A. MOHAMED^{2,4}, HENRIK HAHN¹, IGNACIO G. GONZALEZ-MARTINEZ², KAROLINA WENELSKA³, EWA MIJOWSKA³, BERND BÜCHNER², SILKE HAMPEL², NICO GRÄSSLER², and RÜDIGER KLINGELER¹ — ¹Kirchhoff Institute for Physics, 69120 Heidelberg, Germany — ²Leibniz Institute for Solid State and Materials Research Dresden e.V., 01069 Dresden, Germany — ³Nanomaterials Physicochemistry Department, Faculty of Chemical Technology and Engineering, West Pomeranian University of Technology, 71-065 Szczecin, Poland — ⁴Department of Physics, Faculty of Science, Sohag University, 82524 Sohag, Egypt

We report in the context of lithium-rich antiperovskite cathode materials outstanding electrochemical properties of (Li₂Fe)SeO, which for the first time was synthesized via direct ball-milling. The unique structured material displays a electrochemical cycling performance of 250 mAh g⁻¹ at 0.1 C when used as a cathode in lithium-ion batteries. Comprehensive electrochemical analysis combined with detailed transmission electron microscopy studies reveal that, above 2.5 V, the multi electron storage mechanism involves conversion of (Li₂Fe)SeO to Fe_{1-x}Se_x. Our results furthermore demonstrate the general relevance of our findings to the whole class of antiperovskite cathode materials and present a route to strongly enhance their cell performance by avoiding the degradation path deciphered by our studies.

AKE 2.6 Tue 11:15 TC 006

Effects of Aluminum trifluoride impurities on NMC811 / Graphite Lithium-ion battery performance. — ●SLAHEDDINE JABRI — Institute of Applied Physics, Technische Universität Braunschweig, 38106 Braunschweig, Germany

The effects of aluminum trifluoride (AlF₃) impurities in the electrolyte of full cell lithium-ion batteries has been studied using NMC811/Graphite electrodes. A strong decline of the retention capacity is observed when the cells are cycled at 50 °C in the presence of AlF₃ impurities in the electrolyte. The AlF₃ accelerates the cell degradation by the generation of various compounds during battery operation. The NMC811 cathode and the Graphite anode are characterized with different techniques. Scanning electron microscopy SEM, including cross-section- Focus Ion Beam FIB, Raman spectroscopy and

X-ray photoelectron spectroscopy XPS methods are employed to investigate the effect of the degradation on the electrolyte due to the AlF₃ impurities. We found modified chemical components and morphology of the surface electrolyte interface (SEI) and cathode electrolyte inter-

face (CEI) layers of anode and cathode after cell aging with polymer layers on the both surfaces. Pathways to understand the AlF₃ impact are proposed.