

KFM 15: Materials for Energy Storage (joint session KFM/ CPP)

Chair: Prof. Dr. Theo Scherer (KIT, Karlsruhe)

Time: Wednesday 9:30–12:05

Location: H7

KFM 15.1 Wed 9:30 H7

Hybrid CuCo₂O₄ nanosheets as binder-free supercapacitor electrodes — •ZIDONG WANG^{1,2}, YUDE WANG², HUAPING ZHAO¹, and YONG LEI¹ — ¹Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — ²School of Materials and Energy, Yunnan University, 6500504 Kunming, Peoples Republic of China

CuCo₂O₄ is one kind of pseudocapacitive materials and it has a high theoretical capacitance, but it suffers from poor electrical conductivity. In this work, CuCo₂O₄ nanosheets were directly grown on a conductive skeleton to significantly enhance the conductivity and at the same time reduce the agglomeration of CuCo₂O₄ nanosheets. In addition, the hybrid nanosheet structures also expand the interface and provide more active electrochemical sites, facilitating kinetic processes and electrochemical reactions. The as-prepared CuCo₂O₄ nanosheets on a conductive skeleton were studied as binder-free electrode and exhibited outstanding electrochemical performance with the specific capacitance of 1595 F g⁻¹ at a current density of 1 A g⁻¹ and 85.1% capacitance retention after 4600 cycles. These results indicated that hybrid CuCo₂O₄ nanosheets has great application potential as binder-free electrode in supercapacitors.

KFM 15.2 Wed 9:50 H7

Investigation of K-ion Intercalation and Conversion in Layer Transition Metal Disulfide anode: The case of MoS₂ and WS₂ — •YULIAN DONG, HUAPING ZHAO, and YONG LEI — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Two-dimensional transition metal dichalcogenides (2D-TMDs) have a unique layered structure characterized by weak interlayer van der Waals interaction and strong in-plane covalent bonding. The structure allows the intercalation of guest species in the interlayer space, which shows impressive properties in potassium-ion batteries (PIBs). Thus, various 2D TMDs, including sulfides (MoS₂, SnS₂, WS₂) and selenide (MoSe₂ and VSe₂), have been studied as potential anode materials for PIBs. This work compares the intercalation and conversion of K in MoS₂ and WS₂. Intercalation and conversion process is observed during potassium in MoS₂ in a voltage range of 3.0-0.5V and 0.5-0.01V, respectively. By controlling cut-off voltage, the investigation demonstrated high capacities derived from the conversion, but it destroys the 2D diffusion pathways leading to an unstable cycling span. While the K⁺ storage in WS₂ is governed by the intercalation reaction rather than the conversion reaction. It exhibited a low capacity decay rate at both low and high current densities as well as great rate capability.

KFM 15.3 Wed 10:10 H7

Elucidation of the Pore Formation Mechanism in Hard-Carbon Microspheres — •MARTIN WORTMANN¹, WALDEMAR KEIL², MICHAEL WESTPHAL¹, ELISE DIESTELHORST³, JAN BIEDINGER¹, BENNET BROCKHAGEN³, GÜNTER REISS¹, CLAUDIA SCHMIDT², KLAUS SATTLER⁴, and NATALIE FRESE¹ — ¹Bielefeld University, Bielefeld, Germany — ²Paderborn University, Paderborn, Germany — ³Bielefeld University of Applied Sciences, Bielefeld, Germany — ⁴University of Hawaii, Honolulu, USA

Micro-spherical hydrochar can be carbonized by pyrolysis to produce hard-carbon microspheres with excellent electrochemical properties for the application as anode material in batteries. In this contribution, a temperature-resolved study of the chemical and morphological evolution of saccharide-derived hydrochar during pyrolysis up to 1000°C is presented. By combining a wide range of characterization methods all aspects of the structural transition are examined. The chemical processes occurring both in the bulk and at the surface of the carbon spheres are shown to affect the transition from an amorphous-polymeric to a nanocrystalline carbon-structure. The study focuses on the pore formation mechanism, which is driven by the aggregation of nanometer-sized oxygen-rich clusters at the sphere surface, which disintegrate in a narrow temperature range, leaving behind a mesoporous structure. The revealed molecular mechanisms provide key insights into the pyrolysis of carbonaceous materials.

KFM 15.4 Wed 10:30 H7

Hydrogenation of Pd nanoparticles at the nanoscale with in-situ TEM — •SVETLANA KORNEYCHUK^{1,2}, STEFAN WAGNER¹, GEORGIAN MELINTE², DARIUS ROHLEDER³, PHILIPP VANA³, and ASTRID PUNDT¹ — ¹IAM-WK, Karlsruhe Institute of Technology, Karlsruhe, Germany — ²INT, Karlsruhe Institute of Technology, Karlsruhe, Germany — ³Institute of Physical Chemistry Georg-August-University Göttingen, Göttingen, Germany

Palladium-based nanomaterials play an important role in hydrogen technology. Extreme affinity of palladium to hydrogen is very attractive for various applications. Besides catalysis, Pd nanoparticles can assist in hydrogen delivery into other materials for hydrogen storage through a spill-over process. Pd-based materials are also used as hydrogen purification membranes and hydrogen detectors. The hydrogenation and dehydrogenation process of Pd nanoparticles is hence of high interest in the applications mentioned above. Nanoscale systems reveal significant thermodynamic deviations from the bulk due to higher surface to volume ratio, absence of grain boundaries, different behavior of defects and mechanical stress. In this work, we investigate the behavior of Pd nanoparticles and formation of PdH_x in real time with in-situ H₂-gas TEM. Many applications require operation at elevated temperatures. With the special gas holder from Protochips it is possible to reach pressures up to 1 atmosphere and study the particles at elevated temperatures with the limit of 1000°C. We can observe the local phase change at different temperatures and pressures with the help of spectroscopic and diffraction techniques at the nanoscale.

15 min. break

KFM 15.5 Wed 11:05 H7

Mild-temperature solution-assisted encapsulation of phosphorus into ZIF-8 derived porous carbon as lithium-ion battery anode — •CHENGZHAN YAN¹, SHUN WANG², and YONG LEI¹ — ¹Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany. — ²Key Laboratory of Carbon Materials of Zhejiang Province, Institute of Materials and Industrial Technologies, Wenzhou University, Wenzhou, Zhejiang, 325027, China.

The high theoretical capacity of red phosphorus (RP) makes it a promising anode material for lithium-ion batteries (LIBs). However, the large volume change of RP during charging/discharging imposes an adverse effect on the cyclability, and the rate performance suffers from its low conductivity. Herein, a facile solution-based strategy is proposed to incorporate phosphorus into the pores of MOF-derived carbon hosts under a mild temperature. With this method, the blocky RP is etched into the form of polyphosphides anions (PP, mainly P₅-), making it easily diffuse into the pores of porous carbon hosts. Especially, the indelible crystalline surface phosphorus could be effectively avoided, which is generated in the conventional vapor condensation encapsulation method. Moreover, highly-conductive ZIF-8 derived carbon hosts with any pore smaller than 3 nm are efficient for loading PP and these pores can well alleviate the volume change. Finally, the composite of phosphorus encapsulated into ZIF-8 derived porous carbon exhibits a significantly improved electrochemical performance as LIBs anode.

KFM 15.6 Wed 11:25 H7

Study on Li Ion Diffusion in Li_xV₂O₅ using First Principle Calculations and Kinetic Monte Carlo Simulations — •FABIAN DIETRICH¹, EDUARDO CISTERNAS¹, MARCELO PASINETTI², and GONZALO DOS SANTOS^{2,3} — ¹Universidad de La Frontera, Temuco, Chile — ²Universidad Nacional de San Luis, CONICET, San Luis, Argentina — ³Universidad de Mendoza, Mendoza, Argentina

We study the Li diffusion in Li_xV₂O₅ (0 < x ≤ 1) - a potential cathode material for Lithium ion batteries. Different diffusion pathways in this material in dependence on the Li ion concentration are investigated by applying first-principles calculations. The results are used to obtain the corresponding diffusion coefficients by employing two complementary methodologies: Kinetic Monte Carlo (KMC) simulations and a statistical thermodynamics approach. The KMC simulations for

two different crystal planes give new evidence that the diffusion occurs mainly along the [010] direction, while the corresponding diffusion coefficients show a temperature dependence obeying the Arrhenius' Law. The necessity of the consideration of concentration-dependent barrier heights in the KMC simulations are demonstrated by looking at the significant changes of the concentration-dependence of the diffusion coefficients. The simulated diffusion coefficients of the combined approach show a good quantitative agreement with experimental data reported previously.

KFM 15.7 Wed 11:45 H7

NMR studies of sintering effects on the lithium ion dynamics in $\text{Li}_{1.5}\text{Al}_{0.5}\text{Ti}_{1.5}(\text{PO}_4)_3$ — •PHILIPP SEIPEL¹, EDDA WINTER¹, MICHAEL VOGEL¹, TATIANA ZINKEVICH², SYLVIO INDRIS², BAMBAR DAVASSUREN³, and FRANK TIETZ³ — ¹AG Vogel, Institute for Condensed Matter Physics, Technische Universität Darmstadt, Germany — ²Karlsruhe Institut of Technology, IAM-ESS, Karlsruhe, Germany — ³Forschungszentrum Jülich GmbH, IEK-1, Jülich, Germany

Various NMR methods are combined to study the structure and dynamics of $\text{Li}_{1.5}\text{Al}_{0.5}\text{Ti}_{1.5}(\text{PO}_4)_3$ samples, which were obtained from sintering at various temperatures between 650 °C and 900 °C and show high bulk conductivities up to 5 mS/cm. We use ⁷Li NMR to study the transport mechanism in these glass ceramics [1]. Analysis of ⁷Li spin-lattice relaxation and line-shape changes indicates the existence of two species of lithium ions with clearly distinguishable jump dynamics, which can be attributed to crystalline and amorphous sample regions. An increase of the sintering temperature leads to higher fractions of the fast lithium species with respect to the slow one, but hardly affects the jump dynamics in either of the phases. ⁷Li field-gradient diffusometry reveals that the long-range ion migration is limited by the sample regions featuring slow transport. The high spatial resolution available from the high static field gradients of our setup allows us to observe also the lithium ion diffusion inside the small (< 100 nm) LATP crystallites, yielding a high self-diffusion coefficient of $D=2 \times 10^{-12} \text{ m}^2/\text{s}$ at room temperature. [1]Winter et al., ZPCH, DOI:10.1515/zpch-2021-3109