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List of Posters on AABC_2015_ Mainz, Germany

Poster session **Advanced Materials (25-27 January 2015)**

Amperex Technology Limited/Contemporary Amperex Technology Limited - Novel Additives and Coating Materials Screening from DFT Simulation

BYK-Chemie GmbH - LAPONITE® as Additive in Electrodes of Lithium Ion Batteries

Dong-A University - Properties for Ni-rich NCM Cathode Materials Prepared under Various Synthesis Conditions

Functional Nano Systems (FuN) - Functional Materials for Lithium and Post-Lithium Ion Battery Technologies

Institute of High Performance Computing, Agency for Science, Technology and Research - DFT Modeling of Li Diffusion in V_2O_5 as Cathode Material of Li Ion Batteries

Ioffe Institute - Advanced Solid Electrolytes Based on Alkaline Hydroxides in the Form of Crystalline Hydrates and Eutectics for 240 – 420 K

Karlsruhe Institute of Technology - Performance and Advantages of Sodium-Ion Battery Materials

Korea University - Synthesis of Graphitic Ordered Mesoporous Carbon with Cubic Symmetry and Its Application in Lithium-Sulfur Battery

MATERIALS DESIGN S.A.R.L. - Effect of Grain Boundaries on Li Superionic Conductivity in the Solid Electrolyte LGPS: Understanding and Property Data from Atomistic Simulations

MEET - *Münster Electrochemical Energy Technology* - Beneficial Influence of $LiPF_6$ Hydrolysis Products as Efficient Cathode/Electrolyte Interface Film Forming Additives for High Voltage Lithium-Ion Batteries

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Tim Dagger , University of Muenster

Presenting Tuesday-Thursday

26-27. Jan 2016

ADVANCED MATERIALS

B101. Large-Scale Computational Screening of Electrolyte Materials
Prof. Martin Korth , Ulm University

B102. Pyrotek's Clean Graphitization Process for the Energy Market
Michael J. Sekedat , Pyrotek, Inc.

B103. Highly Conductive Glass-Ceramic Electrolytes for Advanced Lithium Batteries
Wolfgang Schmidbauer , Schott AG

B104. Advanced Solid Electrolytes based on Alkaline Hydroxides in the Form of Crystalline Hydrates and Eutectics for 240 – 420 K
Dr. Yurii Baikov , Ioffe Institute

B105. Atomic Scale Storage Mechanism Studies of the Advanced Anode Materials for Lithium-Ion Batteries
Dr. Xi Wang , National Institute for Materials Science (NIMS)

B106. DFT Modeling of Li Diffusion in V2O5 as Cathode Material of Li-Ion Batteries
Alexander Genest , Institute of High Performance Computing, Agency for Science, Technology and Research

B107. Synthesis of Graphitic Ordered Mesoporous Carbon with Cubic Symmetry and Its Application in Lithium-Sulfur Battery
Min-Seop Kim , Korea University

B108. Novel Additives and Coating Materials Screening from DFT Simulation
Dr. Deven Hu , Amperex Technology Limited/Contemporary Amperex Technology Limited

B109. Preferred Orientation of Li+ Diffusion Matters the Electrochemical Energy of LiMnPO4
Nam Hee Kwon , University of Fribourg

B110. Aqueous Catholyte for Rechargeable Li-Air and Li-Water Batteries

3G

Advanced solid electrolytes based on alkaline hydroxides in the form of crystalline hydrates and eutectics for 240 – 420 K

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The pioneering investigation of the electrochemical activity of certain ionic heterostructures with solid electrolyte $KOH{\cdot}2H_2O$ (T_{melt}=315 K) is due to basic and applied interest in. The special study of different chemical elements of IV group (C, Si, Sn, Pb) as electrodes of electrochemical cells with hydroxide superprotonic conductor as electrolyte has been performed. EMF (1,2 – 1,3 V) and exchange currents (~0,1-1 mA/cm^2) of 'C | $KOH{\cdot}2H_2O$ | TiFe' and 'C | $KOH{\cdot}2H_2O$ | Sn' have been shown to be adequate to work as low-power sources for electronic devices. They are factually batteries from cheap materials without any catalysts. The scientific justification of the opportunity to use such combinations in electrochemical devices has been based on the study of physical nature of different types of heterojunctions. The isotopic shift of the electromotive forces and isotopic (H⇔D) exchange between $TiFeH_x$ - electrodes and $KOH{\cdot}2H_2O$- electrolytes have been studied specially to prove the formation of protonic heterojunction in the electrochemical cell 'C | $KOH{\cdot}2H_2O$ | TiFe'. The metal-protonic heterojunction for 'C | $KOH{\cdot}2H_2O$ | Sn' characterized by enough high exchange current has been studied firstly. The semiconductor-protonic heterojunction in the heterostructure 'C | $KOH{\cdot}2H_2O$ | Si' could be considered as the opportunity of the harmonical combination of small-sized electronic devices with batteries like studied here.

Key words: low-power battery, protonic conductor, graphite, stannum, silicon

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2. Yu.M. Baikov, Solid State Ionics 181 (2010) 545.
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POSTER 4G

Advanced Solid Electrolytes Based on Alkaline Hydroxides in the Form of Crystalline Hydrates and Eutectics for 240-420 K.

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Introduction. Nanostructured eutectics (NaOH+KOH),(KOH+KOH.H_2O), (LiOH+NaOH), (KNH_2+$NaNH_2$) have sufficiently more higher ionic (protonic) conductivity than their "parent" individual compounds. Studying such phenolmena is useful for physics of nano-materials as well as for promising technological application for synthesis and using for energy storage and conversion.

A particular phenomenon was recently discovered, whereby self-organized microheterogeneity of a NaOH+KOH solid eutectic modifies the properties of this proton conductor and thus changes the characteristics of a related "M1|NaOH+KOH|M2" heterostructure. (M1 and M2 are different combinations of electrodes likely Pd, Ti, TiFe, Sn, Ge, C as graphite textile). The basic and applied interest in this phenomenon has related both to a high proton conductivity of the NaOH+KOH solid (!!!) eutectic (10–30 mS/cm). It was several orders of magnitude (!) higher than the conductivity of NaOH and\or KOH individual compounds at moderate temperatures (360–450 K). Moreover the electrochemical activity of such heterostructures was revealed in pioneering special study [1-4]. The much greater conductivity in the indicated temperature range and specific features of the low-frequency impedance spectrum are related to the formation of a microheterogeneous mixture of NaOH and KOH crystals in the course of self-organization accompanying solidification of the eutectic.

Important additional information on the physical nature of structural characteristics of the phase transition was obtained from an analysis of the shapes of peaks in the temperature dependence of the heat capacity of the EA samples measured in the heating and cooling regimes. According to the thermodynamic theory of a self-consistent field in application to shaped smeared first-order phase transitions, numerous fluctuations are localized in a limited volume of the "old" phase so as to form stable nuclei of the

"new" phase called the elementary volumes of the transition. The peaks on the differential scanning calorimetry (DSC) curves are asymmetric, which allows one to assume the existence of at least two components characterized by different values. Using two-component fitting, these values were estimated as ~60–80 nm and ~35–40 nm. The almost two-fold difference is probably related to features of the structure of components forming the EA composition. The assignment of these components to KOH and NaOH requires additional investigation.

Irrespective of the possible variants, these estimates show that the elementary transformation volumes in the region of the first-order phase transition contain up to 1000 crystal unit cells. This corresponds to a quite large domain, the further growth of which depends on the subsequent treatment of a sample. In concluding, it should be noted that investigations described above form an approach to the search for and creation of nano-heterogeneous ionic conductors employing the phenomenon of self-organization in eutectic mixtures.

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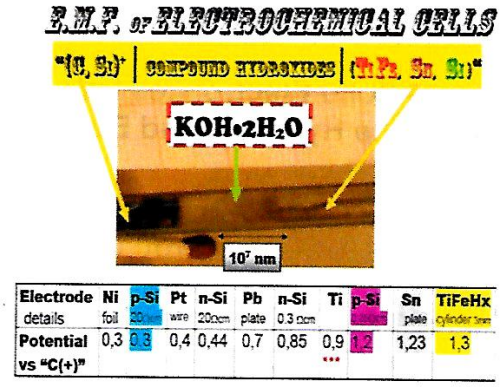

The special study on proton transport in all four eutectics (i.d. includingKOH+KOH.H_2O, LiOH+NaOH, KNH_2+$NaNH_2$) will be presented and discussed from points of physics of solid electrolytes in nanoheterogeneous state as well as the properties of electrochemical devices for energy conversion and storage.

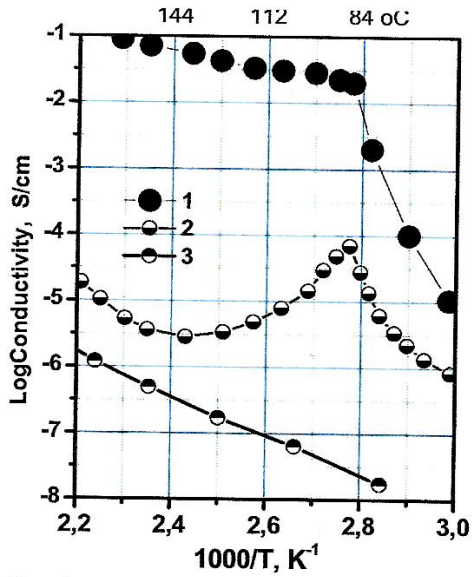

Fig.1. Self-organized eutectic (3) NaOH(1)-KOH(2) as protonic conductors (3) have more higher conductivity than both parents .