AKE 3: Poster

Time: Tuesday 12:00–14:00 Location: Poster C

AKE 3.1 Tue 12:00 Poster C

Das Problem der Reinheit von flüssigem Wasserstoff bei der Verwendung als Kraftstoff — •Artemii Yakushev — Moscow, Russia

Flüssiger Wasserstoff ist ein umweltfreundlicher und energieintensiver Kraftstoff. Damit es jedoch allgemein und sicher verwendet wird, muss die Kraftstoffqualität hoch sein.

Eine direkte Analyse von flüssigem Wasserstoff ist nicht möglich, daher werden die verdampften Proben analysiert. Hier gibt es unter anderem ein Problem: nur Helium und Neon befinden sich im gasförmigen Zustand bei einer Temperatur unter -252°C (das ist die Temperatur des flüssigen Kraftstoffs), und die Löslichkeit der anderen Hauptverunreinigungen, die sich im festen oder flüssigen Aggregatzustand befinden, ist sehr gering (etwa 1*10-7-1*10-6 %). Auf dieser Weise wird bei der Verdampfung von Wasserstoff werden Verunreinigungen konzentriert, die chemische Zusammensetzung des Kraftstoffs ändert sich.

In dieser Arbeit, um das Verhalten der Verunreinigung bei verschiedenen Kraftstoffmanipulationen leichter zu verfolgen, betrachten wir folgenden Klassifizierungen: nach dem Aggregatzustand, in dem sich die Verunreinigung in verflüssigtem Wasserstoff befindet und in dem sie beim Erhitzen des Kraftstoffs gelangen wird.

Durch diese beiden Parameter kann das Verhalten den Gruppen der Verunreinigung verfolgt werden.

AKE 3.2 Tue 12:00 Poster C

Modernization of the Compressed Air Supply System for Gas Compressor Units (GPA) — •Sergey Kalinin — Moscow, Russia

The goal is to reduce the operational costs of a gas compressor unit. A design involving a block-container automated unit with a gas turbine drive of the NK-16-18STD type with an 18 MW power output, a centrifugal gas compressor reaching a final pressure of 9.9 MPa and a compression ratio of 2.32, equipped with a rotor featuring magnetic bearings and end gas-dynamic seals, has been considered.

The compressed air delivery system for the GPA's needs has been examined. An alternative air delivery system with the required parameters has been reviewed. A technological solution and structural design for the alternative air delivery system have been proposed. Calculations for the technological and structural parameters of the GPA sealing system have been carried out. Economic justification for the project to modernize the compressed air delivery system is provided. This research was made in the Strategic Academic Leadership program.

AKE 3.3 Tue 12:00 Poster C

EXPERIENCE IN USING TITANIUM BLADES — •Vasilisa Maslova — Moscow, Russia

Titanium and its alloy VT6 have been studied, the temperature of polymorphic transformation has been determined by the method of trial hardening, the two-phase composition of the alloy has been investigated, and its microstructure has been examined. The dependence of the content of the alpha phase on the hardening temperature at the same holding time has been revealed. In addition, statistical processing of supplier data on yield strength, ultimate tensile strength, elongation, reduction in area, impact toughness (KCU), and content of alpha phase of stamped blade blanks has been conducted. Histograms of the distribution of final mechanical properties have also been obtained, leading to a conclusion about the stability of the manufacturing technology. This research was made in the Strategic Academic Leadershop program.

AKE 3.4 Tue 12:00 Poster C

Applying self-driving car technology to life — •Hong Duc Phan — Moscow, Russia

In the realm of automotive technology today, autonomous driving technology is revolutionary. The purpose of driving technology research and development is to make driving more stress-free and relaxing for drivers. Utilizing satellite signals, the vehicle's surrounding sensors are combined to handle operational circumstances. Improve the car's comfort and safety. The article focuses on the potential applications of autonomous vehicle technology. But more investigation is required to boost user dependability.

AKE 3.5 Tue 12:00 Poster C

Metal Halide Perovskites as anode materials in hybrid organic inorganic lithium ion batteries — •Tom Wickenhäuser[1], Shangpu Liu[2], Lennart Singer[1], Felix Deschler[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg, Germany — [2]Physikalisch-Chemisches Institut, Heidelberg, Germany

We report on the characterisation of metal halide perovskites as electrode materials in hybrid organic-inorganic lithium-ion batteries. In particular, $MAPbBr_3$, one dimensional $EAPbI_3$ and two lead-free perovskites $CsMnBr_3$ and $EA_4Bi_2Br_{10}$ are investigated as anode material for lithium-ion batteries. Cyclic voltammetry as well as galvanostatic cycling measurements were performed to elucidate the electrochemical reaction mechanism with a special focus on the ionic and electronic transport characteristics. Additional investigations on the influence of different electrolytes on the electrochemical performance revealed an improved cycling stability for 1M LiTFSI in DOL/DME (1:1) compared to 1M $LiPF_6$ in EC/DMC (1:1). In the context of these studies; promising first cycle capacities of 560 mAh g^{-1} for $MAPbBr_3$, 440 mAh g^{-1} for $EAPbI_3$, 330 mAh g^{-1} for $EA_4Bi_2Br_{10}$ and 201 mAh g^{-1} for $CsMnBr_3$ were achieved.

AKE 3.6 Tue 12:00 Poster C

Application of the Miller cycle to the diesel engine to improve its environmental performance — •Yuriy Kochanov — Russia, Moscow

This work demonstrates the application of the Miller cycle to the diesel engine 12FB26,5/31 to improve its environmental performance. Two methods of implementing the Miller cycle, "early" and "late," are investigated, and the choice of one method is justified. IVC and EVO angles are selected to implement the chosen method of the Miller cycle. The problem of reducing engine power during the implementation of the Miller cycle is solved by compensating with increasing of the degree of pressure increase in the compressor. Gas recirculation is applied in conjunction with the Miller cycle. Gas distribution phases, degree of pressure increase in the compressor, and degree of recirculation are selected using numerical modeling in a one-dimensional approach. All parameters are selected through single-factor or two-factor optimization based on emission of harmful oxides and particulate matter. As a result of this work, the engine's operating process meets environmental requirements for emissions of NOx, SOx, CO2, and emission of solid particles. This research was made in the Strategic Academic Leadership program.

AKE 3.7 Tue 12:00 Poster C

Simulation of noise dampening during construction of offshore windparks — •Tobias Bollig[1,2], Angela Thränhardt[1], Thomas Blaudeck[2,4], and Fabian Teichert[2,3,4] — [1]Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany — [2]Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz Universitity of Technology, Chemnitz, Germany — [3]Center for Microtechnologies, Chemnitz University of Technology, Chemnitz, Germany — [4]Fraunhofer Institute for Electronic Nano Systems (ENAS), Chemnitz, Germany

Because of the growing relevance of offshore windparks due to the "Energiewende", the regulations of building these giant wind turbines are more important than ever. The construction of the foundations of the wind turbines creates huge sound emissions for the surrounding marine life. To dampen these negative effects, there are different ways to reduce the sound emission during construction. This work presents a new simulation approach of the sound dampening characteristics of the most commonly used technique called big bubble curtain. We simulate them using the finite element method in the open source software "Elmer". Previous investigations focused on 3D simulations of the bubble curtain as a heterogeneous medium. We implement a numerical calculation based on the theory of the effective medium to deliver an extremely time-efficient method, especially considering a wide range of parameters to be investigated in future projects. First results show that 2D simulations achieve roughly the same sound dampening as is available from data sheets of industrial used bubble curtains.

AKE 3.8 Tue 12:00 Poster C

Twist angle-dependent electronic and optical properties of transition metal dichalcogenide (TMD) Van der Waals het-

erostructures — •Neelam Gupta, Saurav Sachin, Puja Kumari, Shivani Rani, and Soumya Jyoti Ray — Department of Physics, Indian Institute of Technology Patna, Bihta 801106, India

Recent research has focused on transition metal dichalcogenides(TMDs) based heterostructures due to their potential applications in electronics and optoelectronics. This study investigates the impact of twist angles on the electronic, and optical characteristics of vertically stacked heterostructures based on transition metal dichalcogenides, namely MoSe2/WSe2, WS2/WSe2, MoSe2/WS2, and MoS2/WSe2, and a thorough comparison is done among these heterostructures. The absence of negative frequency in the phonon dispersion curve and low formation energy affirm their structural and thermodynamic stability. The calculations are performed using the first-principles- based density functional theory (DFT) considerations. Beautiful Moir'e patterns are formed due to the relative rotation of the layers as a consequence of the superposition of the periodic structure of TMDs on each other. Twist engineering allows the modulation of bandgaps and phase change from direct to indirect band gap semiconductors. The high optical absorption in the visible range spectrum makes these twisted heterostructures promising candidates in photovoltaic applications.

AKE 3.9 Tue 12:00 Poster C

Comparative Study of the Interfacial Stability at the Anode Site in Lithium and Sodium All-Solid-State Batteries Utilizing Density Functional Theory — Sebastian Utz[1,2] and •Doreen Mollenhauer[1,2] — [1]Institute of Physical Chemistry, Justus-Liebig University Giessen, Germany — [2]Center for Materials Research (LaMa), Justus-Liebig University Giessen, Germany

Improving and understanding the stability of the anode/electrolyte interface is one of the key challenges in the design of emerging high energy density batteries. One of these emerging battery types is the all-solid-state battery, which utilizes a lithium metal anode and promises, among other benefits, large improvements in energy density. However, it is particularly difficult to obtain experimental information at the solid/solid anode interface. Here, a theoretical study at density functional theory (DFT) level of theory has been carried out to investigate the interfacial stability of a high-capacity lithium metal anode in contact with a thiophosphate solid electrolyte and the analogous post-lithium sodium metal system, commonly regarded as a more sustainable alternative. Similarities and differences between the two systems are explored and discussed.

AKE 3.10 Tue 12:00 Poster C

The stable nature of the decomposition interface in LiPON electrolyte with lithium anode — •Kangli Wang and Doreen Mollenhauer — Gießen/DE, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 17, 35392 Gießen

All-solid-state batteries (ASSBs) have the potential to offer several advantages over the currently used liquid Li-ion battery technology. To improve the cell properties of ASSBs, it is to crucial to understand the interfaces between the Li-metal anode and the solid electrolytes (SE). Experimental efforts at the Li/LiPON interface revealed the decomposition products Li_2O, Li_3N, Li_3P, and Li_3PO_4. Nevertheless, there is still a lack of deep understanding the Li/LiPON interface, particularly with respect to the interfacial decomposition and reconfiguration.

To take a step towards understanding ASSB interfaces, we explore in detail the role of different interfacial compositions and morphologies caused by decomposition reactions of the Li/LiPON interface. We investigate and characterize all possible occurring Li/LiPON interfaces (including Li/Li_2O, Li/Li_3N, Li/Li_3P and Li/Li_3PO_4) and LiPON/LiPON interfaces (including Li_2O/Li_3N, Li_2O/Li_3P, Li_2O/Li_3PO_4, Li_3N/Li_3P, Li_3N/Li_3PO_4 and Li_3P/Li_3PO_4) using density functional theory (DFT) calculations. We believe that our study provides a fundamental understanding to guide the future design of solid electrolytes and interfaces in ASSBs.

AKE 3.11 Tue 12:00 Poster C

First principles calculations of borides alloy — •Jiangming Cao — Helmut-Schmidt University, Holstenhofweg 85, 22043 Hamburg, Germany

In the preparation of hydrogen storage materials, boron element is inevitably introduced and thus ternary alloys are produced. We need to explore which alloys are easy to form and which borides affect the properties of hydrogen storage materials. The basic working on is trying to change lattice constant of TiB2 to match the lattice constant of MgB2 by alloying into TiB2, finding alloying part of this TiB2. A range of elements near Ti in the periodic table as possible candidates, when initially for elements that crystallized in the same structures TiB2. Then some boride-like structures were found, exhibiting larger lattice constant than TiB2. The basic purpose is to alloy TiB2 with one of the other elements (Sc, Y, Zr, Hf, Nb and Ta). The predicted (Ta:Ti)B2 alloy exhibited novel ternary ground state that break the convex hull and low zero-temperature formation energy cover the entire range of considered concentration. When the composition is Ta1/3Ti2/3B2, this alloy composition should be achievable easily, due to the lowest formation energy. From the Ta-rich to Ti-rich side, 9 ternary borides breaking the convex-hull are advantage over other corresponding concentration. Such as Ta1/8Ti7/8B2, Ta2/9Ti7/9B2, Ta1/3Ti2/3B2, Ta4/9Ti5/9B2, Ta1/2Ti1/2B2, Ta2/3Ti1/3B2, Ta7/9Ti2/9B2, Ta5/6Ti1/6B2, and Ta8/9Ti1/9B2, are predicted here.