Working Group on Energy
Arbeitskreis Energie (AKE)

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Affordable, reliable and climate protecting energy supply is indispensable for a real sustainable development. Physics, engineering and many more sciences contribute to this objective. The following 3 sessions on concepts and technologies, energy supply, and perspectives for the future present two invited talks and 22 submitted contributions. They reflect needs for enhancing a sound energy system, including societal and political questions.

Overview of Invited Talks and Sessions

(Lecture hall TC 006; Poster C)

Invited Talks

AKE 1.1	Mon	15:00–15:30	TC 006	**Unser Energiesystem der Zukunft: Neue Hoffnung für den Klimaschutz** — •Wolfgang Eberhardt
AKE 2.1	Tue	9:30–10:00	TC 006	**Concepts for combining concentrating solar mirrors with PV modules** — •Moritz Ruhwedel, Kai Gehrke, Eckhard Lüpfert, Florian Sutter, Peter Heller, Robert Pitz-Paal

Sessions

AKE 1.1–1.7	Mon	15:00–17:15	TC 006	**Innovative Energy Transformation Concepts**
AKE 2.1–2.6	Tue	9:30–11:30	TC 006	**Processes and Materials for Energy Technologies**
AKE 3.1–3.11	Tue	12:00–14:00	Poster C	**Poster**

AKE 1: Innovative Energy Transformation Concepts

Time: Monday 15:00–17:15 Location: TC 006

Invited Talk AKE 1.1 Mon 15:00 TC 006

Unser Energiesystem der Zukunft: Neue Hoffnung für den Klimaschutz — •Wolfgang Eberhardt — DESY, Notkestr. 85, 22607 Hamburg

Seit der überwältigenden Zustimmung zum Pariser Klima-Abkommens besteht allgemeiner Konsens darüber, dass unser Energiesystem von der derzeitigen Basis fossiler Brennstoffe zu einem nachhaltigeren System auf Basis erneuerbarer Energien geändert werden muss. Politiker überbieten sich schnell mit Versprechen, die CO2- Emissionen zu reduzieren, ohne anzugeben, wie dies erreicht werden soll. Es ist jedoch ein Energiesystem möglich, das weitgehend auf erneuerbaren Energien und Strom basiert, ein System, das die Auswirkungen des Klimawandels umkehrt, Gesundheitsbelastungen durch Umweltverschmutzung beseitigt und dennoch den Anforderungen an Verkehr, Industrie und Gebäude in der Gesellschaft der Zukunft trotz der weltweit wachsenden Bevölkerung gerecht wird, erschwinglich ist und wirtschaftliches Wachstum ermöglicht. Es wird gezeigt, wie dies bis 2050 erreicht werden kann.Es beruht im wesentlichen darauf, daß der CO2 Gehalt der Atmosphäre zurück geht, sobald etwa 50% der heutigen CO2 Emissionen eingespart werden wenn wir die natürlichen Senken in Pflanzen und Ozeanen korrekt in die Modelle einbeziehen.

AKE 1.2 Mon 15:30 TC 006

Numerical simulations of the screen printing process for solar cell metallization — •Tom Hoger, Marius Singler, Andreas Lorenz, Florian Clement, and Andreas Bett — Fraunhofer ISE, Germany, Freiburg im Breisgau

The metallization of silicon wafers is an essential part of the production process for Si-solar cells. Due to its robust and costeffective production capability, flatbed screen printing is by far the most used metallization technology nowadays. In order to achieve maximum efficiency and optimum material usage, the parameters of the printing process must be adjusted to the print layout. The huge interdependent parameter space of flatbed screen printing makes it difficult to predict the optimal settings. To this day, these parameters are still chosen based on experience and by iterative manner until a satisfying print result is achieved.

Another approach to handle the complexity of choosing the correct parameters is the use of Computational Fluid Dynamics (CFD) simulations. The successful setup of a CFD simulation could prevent cost-intensive iteration procedures and propose the right choice of parameters via numerical simulations. With the help of CFD simulations, the influence of structural changes in the screen on the flow of the shear-thinning paste is studied. Therefore, a model is built from scratch representing the different process steps of screen printing. Finally the results of different screen structures and paste models are compared and verified with experimental print results.

AKE 1.3 Mon 15:45 TC 006

Photovoltaic efficiency of transition metal dichalcogenides thin films by ab initio excited-state methods — Enesio Marinho Jr[1], Cesar Villegas[2], •Pedro Venezuela[3], and Alexandre Rocha[4] — [1]Departamento de Física e Química, Universidade Estadual Paulista (UNESP), Av. Brasil, 56, Ilha Solteira, 15385-007 São Paulo, Brazil. — [2]Departamento de Ciencias, Universidad Privada del Norte, Lima 15434, Peru — [3]Instituto de Física, Universidade Federal Fluminense (UFF), Av. Gal. Milton Tavares de Souza, s/n, 24210-346 Niterói, Rio de Janeiro, Brazil. — [4]Instituto de Física Teórica, Universidade Estadual Paulista (UNESP)

Transition metal dichalcogenides (TMDCs) have garnered significant interest in optoelectronics, owing to their scalability and thickness-dependent electronic and optical properties. In particular, thin films of TMDCs could be used in novel photovoltaic devices. In this work, we employ ab initio many-body perturbation theory within GW-BSE approach to accurately compute the optoelectronic properties of thin films of 2H-TMDCs composed of Mo, W, S, and Se.

Subsequently, we evaluate their photovoltaic performance including exciton recombination effects, and show this is a key ingredient. We obtain efficiencies of up to 29 % for a 100-nm thick film of WSe2, thus providing an upper limit. We also include other phenomenological recombination mechanisms that could be present in current samples. This slightly reduces efficiencies, indicating that even with current synthesis technologies, there is still potential for further enhancement of TMDCs performance in photovoltaic applications.

AKE 1.4 Mon 16:00 TC 006

On the theoretical framework for meniscus-guided manufacturing of large scale OPV modules — •Fabian Gumpert[1], Annika Jannssen[1,2,3], Christoph J. Brabec[2,3], Hans-Joachim Egelhaaf[2,3], Jan Lohbreier[1], and Andreas Distler[2,3] — [1]Technische Hochschule Nürnberg Georg Simon Ohm — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg — [3]Helmholtz Institut Erlangen-Nürnberg

For the manufacturing of thin films of solution-processable organic semiconductors, e.g. for organic photovoltaics (OPV), meniscus guided-coating techniques are the method of choice for large scale industrial applications. However, the process requires an in-depth understanding to control the resulting film thickness. We propose an analytical expression to describe the layer thickness manufactured with a trapezoidal shaped applicator. Thus, the theoretical expression has the potential to reduce time and resource consuming experiments (e.g. maximum efficiency). For OPV, uniform layers with predefined thicknesses are necessary to achieve desired layer characteristics. For large surfaces, the significant loss of coating fluid beneath the applicator during the coating process leads to decreasing layer thicknesses with increasing coating distances. Here, we propose that an acceleration of the applicator during the process can compensate the liquid loss and thus, leads to a uniform predefined layer thickness. Expressions, which are based on theory and CFD simulation, to describe the velocity as a function of time are derived and validated by experimental data.

15 min. break

AKE 1.5 Mon 16:30 TC 006

Graphite intercalation of AlF_3: in-plane and interlayer interactions — •Sindy J. Rodriguez[1], Adriana E. Candia[1], Igor Stanković[2], Mario C.G. Jr. Passeggi[1], and Gustavo Ruano[3] — [1]Instituto de Física del Litoral, Consejo Nacional de Investigaciones Científicas y Técnicas y Universidad Nacional del Litoral (IFIS-Litoral, CONICET-UNL) Santa Fe, Argentina — [2]Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, 11080 Belgrade, Serbia — [3]Centro Atómico Bariloche, Comisión Nacional de Energía Atómica (CNEA), Bariloche, Argentina

The electrolyte intercalation mechanism facilitates the insertion/extraction of charge into the electrode material in rechargeable batteries. Aluminium fluoride (AlF_3) has been used as an electrolyte in rechargeable aluminium batteries, the intercalation mechanism of this neutral molecule in graphite is so far unknown. In this work, we combine STM in UHF conditions, DFT calculations, and large-scale MD simulations to reveal the mechanism of AlF_3 intercalation. We report the formation of AlF_3 molecules clusters between graphite layers, their self-assembly by graphene buckling-mediated interactions, and explain the origin and distribution of superficial *blisters* in the material. **Reference** [1] S. J. Rodríguez et al, ACS Appl. Nano Mater. 18, 16977-16985 (2023).

AKE 1.6 Mon 16:45 TC 006

AI-Driven In-situ Experimental Spectroscopy Analysis in Energy Chemistry — •Haobo Li — The University of Adelaide

Single-atom catalysts (SACs) offer significant potential across various applications, yet our understanding of their formation mechanism remains limited. Notably, the pyrolysis of zeolitic imidazolate frameworks (ZIFs) stands as a pivotal avenue for SAC synthesis, of which the mechanism can be assessed through infrared (IR) spectroscopy. However, the prevailing analysis techniques still rely on manual interpretation. Here, we report a artificial intelligence (AI)-driven analysis of the IR spectroscopy to unravel the pyrolysis process of Pt-doped ZIF-67 to synthesize Pt-Co3O4 SAC. Demonstrating a total Pearson correlation exceeding 0.7 with experimental data, the algorithm provides correlation coefficients for the selected structures, thereby confirming crucial structural changes with time and temperature, including the decomposition of ZIF and formation of Pt-O bonds. These findings reveal and confirm the formation mechanism of SACs. As demonstrated, the

integration of AI algorithms, theoretical simulations, and experimental spectral analysis introduces an approach to deciphering experimental characterization data, implying its potential for broader adoption.

AKE 1.7 Mon 17:00 TC 006

Simulation of an electromagnetic vibration energy harvester and possibilities of increasing efficiency and scalability — •Eugen Vambolt — Technische Hochschule Nürnberg Georg Simon Ohm

To ensure the reliability of infrastructures such as roads, bridges, buildings, etc., they must be constantly monitored. To this end, networks of wireless sensor nodes are increasingly being used, which can be operated autonomously through the use of energy harvesters. Energy harvesters are small modules that can convert ambient energy such as light, vibration or temperature differences into electrical energy. The use of Vibration Energy Harvesters (VEH) is therefore ideal for applications that are associated with vibrations or shocks. There are several types of VEH, depending on how they work. One type of VEH is based on electromagnetic induction. Although there are different designs, the principle is the same: a magnet set in oscillation by vibrations or shocks induces an electrical voltage in a fixed coil, which can be used to supply the sensor nodes with energy through the use of low-power electronics. By changing the topological and material properties of the individual components, it is possible to increase performance and efficiency. In this thesis, a model of the electromagnetic vibration energy collector is constructed and a multiphysical simulation is carried out. In addition, a possibility of scaling by varying the design and materials will be demonstrated.

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 Gehrke[3], Eckhard Lüpfert[1], Florian Sutter[1], Peter Heller[1], and Robert Pitz-Paal[1,2] — [1]DLR (German Aerospace Center) Institute of Solar Research, Linder Höhe, 51147 Köln, Germany — [2]RWTH Aachen University, Chair of Solar Technology, Linder Höhe, 51147 Köln, Germany — [3]DLR (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-Ilica[1], Dan Zhao[1], Cherie Hsu[1], Erisa Saraci[1], Moritz Wolf[1], Felix Studt[1], Michael Cleays[2], Denzil Moodley[3], and Jan-Dierk Grunwaldt[1,4] — [1]IKFT-KIT / Eggenstein-Leopoldshafen / Germany — [2]University of Cape Town / South Africa — [3]Sasol South Africa / South Africa — [4]ITCP-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 heterostructure 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 Walls hetero-structure made of conducting 2D $NbSe_2$ -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 V_2C MXene as anode materials for Li-Ion batteries — •Tobias König[1], Peng Guo[1,2], Tom Wickenhäuser[1], Lennart Singer[1], Peter Comba[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institut für Physik, Universität Heidelberg, Im Neuenheimer Feld 227, D-69120 Heidelberg, Germany — [2]Anorganisch 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 V_2C 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 V_2C. 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 V_2C 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 V_2C 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 $(Li_2Fe)SeO$ — •Lennart Singer[1], M.A.A. Mohamed[2,4], Henrik Hahn[1], Ignacio G. Gonzalez-Martinez[2], Karolina Wenelska[3], Ewa Mijowska[3], Bernd Büchner[2], Silke

Hampel[2], Nico Gräßler[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, 69120 Heidelberg, Germany — [2]Leibniz Institute for Solid State and Materials Research Dresden e.V., 01069 Dresden, Germany — [3]Nanomaterials Physicochemistry Department, Faculty of Chemical Technology and Engineering, West Pomeranian University of Technology, 71-065 Szczecin, Poland — [4]Department 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 $(Li_2Fe)SeO$, 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 $(Li_2Fe)SeO$ 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 interface (CEI) layers of anode and cathode after cell aging with polymer layers on the both surfaces. Pathways to understand the AlF3 impact are proposed.

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 Leadership 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 heterostructures — •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.