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.