

## KFM 21: Functional semiconductors for renewable energy solutions (joint session HL/KFM)

Time: Wednesday 15:00–18:30

Location: H36

KFM 21.1 Wed 15:00 H36

**A facile freeze-thaw ultrasonic assisted circulation method of graphite flakes prepared by anode graphite from spent lithium-ion batteries** — •YU QIAO<sup>1,2</sup>, ZHONGHAO RAO<sup>3,4</sup>, HUAPING ZHAO<sup>1</sup>, and YONG LEI<sup>1</sup> — <sup>1</sup>Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — <sup>2</sup>School of Electrical and Power Engineering, China University of Mining and Technology, 221116, Xuzhou, China — <sup>3</sup>School of Energy and Environmental Engineering, Hebei University of Technology, 300401, Tianjin, China — <sup>4</sup>Hebei Key Laboratory of Thermal Science and Energy Clean Utilization, Hebei University of Technology, 300401, Tianjin, China

Lithium-ion batteries (LIBs) have been widely employed in fast-growing mobile devices, stationary storage devices and electric vehicles. However, limited by particular service life, the booming increase in LIBs production will result in a large retirement wave. As the most common anode material in LIBs, waste graphite has also developed into a mode of high production capacity with the retirement of spent LIBs. Anode graphite (AG) of spent LIBs has the characteristics of large layer spacing and ease of being intercalated due to the reduced interlamination force after repeated charge and discharge cycles. This study presents a facile freeze-thaw ultrasonic-assisted circulation method to prepare two-dimensional low-layer graphite flakes (GFs) using AG from spent LIBs. The results indicate that the freeze-thaw ultrasonic-assisted circulation method is feasible for preparing two-dimensional laminar materials.

KFM 21.2 Wed 15:15 H36

**How could the heating process reduce the crystal damage of semiconductors?** — •KHALID LAHMIDI, JALE SCHNEIDER, ANDREAS BRAND, SEBASTIAN RODER, and ANDREAS BETT — Fraunhofer Institute for Solar Energy Systems, Heidenhofstr. 2, 79110 Freiburg, Germany

Laser material processing can no longer be imagined away from the production chains in semiconductor industries. While being a precise, fast and wear-free processing tool, high intensity laser irradiation can also induce damage within the material, e.g. crystal damage, compromising the device quality. However, this damage can partly be healed or even prevented by an accompanying (laser) heating process.

In our laser lab, we built up a flexible laser heating setup with a spatial light modulator (SLM) as the core element. The setup allows to locally heat work pieces with different beam shapes with an intensity up to 220 W/cm<sup>2</sup> employing a cw-infrared laser source. Current research focuses on the temperature distribution in dependence of beam shape and beam dwell time on a specific position. Comsol based simulations support the experiments. Eventually, the heating beam will be overlaid to the process beam in use cases such as laser contact opening at lowered ablation thresholds or laser metal bonding for solar cell manufacturing. The damage after laser process with and without heating will be analyzed via microscopy.

KFM 21.3 Wed 15:30 H36

**Energy landscape of the Boron and Indium single-atom defects in Silicon calculated by DFT** — •AARON FLÖTOTTO, WICHARD BEENKEN, and ERICH RUNGE — Institut für Physik, Technische Universität Ilmenau, Weimarer Str. 32, 98693 Ilmenau, Germany

The III group elements Boron and Indium form not only substitutional defects, which are important as electron acceptors, but also interstitial defects. Different configurations are possible for a single impurity atom: (i) the impurity atom on an interstitial site, (ii) a substitutional impurity near a single interstitial Si atom, or (iii) the impurity and one Si atom form a pair of interstitials around an empty lattice point. We calculated within DFT the stable configurations of these defects for the Si:B and the Si:In system. We utilized the Nudged Elastic Band algorithm for finding minimal paths between these energetic minima in order to explore the energy landscape and to derive transition probabilities. The results are discussed with respect to the dynamical model suggested by K. Lauer et al. [1] for the explanation of PL-spectra of In-doped Si. [1] Lauer, K.; Möller, C.; Schulze, D. & Ahrens, C.; AIP Adv. 5 (2015) 017101

KFM 21.4 Wed 15:45 H36

**Effects of Defects on the Optoelectronic Properties of Ta<sub>3</sub>N<sub>5</sub> Thin Films** — •LUKAS M. WOLZ, GABRIEL GRÖTZNER, LAURA I. WAGNER, IAN D. SHARP, and JOHANNA EICHHORN — Walter Schottky Institut, Technische Universität München

For photoelectrochemical energy conversion, metal nitride semiconductors have the potential to overcome several limitations associated with the more intensively investigated class of metal oxides. Among these materials, Ta<sub>3</sub>N<sub>5</sub> is especially promising, possessing a bandgap of ~2.2 eV and effective long-range charge transport. However, the (opto)electronic and photoelectrochemical properties of Ta<sub>3</sub>N<sub>5</sub> photoelectrodes are often dominated by defects, such as oxygen impurities, nitrogen vacancies, and low-valent Ta cations. To identify the impact of such defects on the material properties, we prepare Ta<sub>3</sub>N<sub>5</sub> via two different synthetic routes. As precursor, Ta<sub>x</sub>N<sub>y</sub> and Ta<sub>x</sub>O<sub>y</sub> thin films were deposited by magnetron sputtering and were subsequently annealed at high temperatures in NH<sub>3</sub> to form Ta<sub>3</sub>N<sub>5</sub>. Both films are homogenous and reveal the formation of phase-pure orthorhombic Ta<sub>3</sub>N<sub>5</sub>. Compared to nitride-derived Ta<sub>3</sub>N<sub>5</sub>, the oxide-derived films are characterized by higher structural disorder as well as higher oxygen and lower nitrogen concentrations. Despite these higher defect concentrations, the oxide-derived Ta<sub>3</sub>N<sub>5</sub> films exhibit improved stability under photoelectrochemical operation conditions, though both films show similar photoelectrochemical performance. The improved understanding of defect properties and their impact on PEC stability provides a path to tailored optimization of photoelectrode properties.

KFM 21.5 Wed 16:00 H36

**Investigation of various quenching materials on the P-line** — •DOMINIK BRATEK, KATHARINA PEH, KEVIN LAUER, AARON FLÖTOTTO, DIRK SCHULZE, and STEFAN KRISCHOK — Institut für Physik, Technische Universität Ilmenau, Weimarer Str. 32, 98693 Ilmenau, Germany

Solar-grade Si shows degradation effects and a lowering of the charge carrier lifetimes after illumination [1]. For In implanted Si this effect was shown to be connected to the P-line in photoluminescence spectra [2]. This P-line can furthermore be influenced by applying a strong quenching after an anneal. The intensity of the P-line increases by several orders of magnitude depending on the cooling rate [3]. In this contribution we investigate the influence of four different quenching liquids on the P-line. From an experimental point of view we discuss the applicability of each used liquid in consideration of P-Line intensity and probe integrity. [1] C. Möller and K. Lauer, Physica Status Solidi (RRL) 7, 461 (2013). [2] K. Lauer, C. Möller, D. Schulze, and C. Ahrens, AIP Advances 5, 017101 (20125). [3] M. L. W. Thewalt, U. O. Ziemelis, and P. R. Parsons, Solid State Communications 39, 27 (1981).

KFM 21.6 Wed 16:15 H36

**Simulation of the reaction kinetics of the A<sub>S<sub>i</sub></sub>-Si<sub>i</sub>-defect** — •KEVIN LAUER<sup>1,2</sup>, KATHARINA PEH<sup>2</sup>, WICHARD BEENKEN<sup>2</sup>, ERICH RUNGE<sup>2</sup>, and STEFAN KRISCHOK<sup>2</sup> — <sup>1</sup>CIS Forschungsinstitut für Mikrosensorik GmbH, Konrad-Zuse-Str. 14, 99099 Erfurt, Germany — <sup>2</sup>TU Ilmenau, Institut für Physik und Institut für Mikro- und Nanotechnologien, 98693 Ilmenau, Germany

Light-induced degradation (LID) is a severe problem for silicon photo-sensitive devices like solar cells and photo detectors. LID reaction kinetics may be explained by the A<sub>S<sub>i</sub></sub>-Si<sub>i</sub>-defect model. [1] This model consists of seven states. The transitions between these states are assumed to be first order equilibrium reactions, which can be mathematically treated by a system of linear differential equation. [1] This is numerically solved and compared to the LID cycle using well-known together with some estimated reaction constants.

[1] K. Lauer, C. Möller, C. Tessmann, D. Schulze, and N. V. Abrosimov, "Activation energies of the In<sub>S<sub>i</sub></sub>-Si<sub>i</sub> defect transitions obtained by carrier lifetime measurements", physica status solidi (c), vol. 14, no. 5, p. 1600033, 2017.

30 min. break

KFM 21.7 Wed 17:00 H36

**Exploring Zirconium-doped Tantalum Nitride as a Photoan-**

**ode for Solar Energy Conversion** — ●OLIVER BRUNE, LAURA I. WAGNER, VERENA STREIBEL, and IAN D. SHARP — Walter Schottky Institut and Physics Department, Technical University of Munich, Am Coulombwall 4, 85748 Garching, Germany

Solar water splitting could pave the way to carbon-free hydrogen production as it allows for direct transformation of sunlight into chemical energy. While the oxygen evolution reaction is a crucial step in generating green hydrogen, there remains a lack of semiconductor photoanode materials that can simultaneously fulfill three key requirements: long-term chemical stability, high photocarrier extraction efficiencies, and appropriate bandgap for harvesting solar radiation. Nevertheless, among the various materials that have been investigated, the transition metal nitride Ta<sub>3</sub>N<sub>5</sub> offers significant promise as an efficient n-type photoanode. Building upon this established material, we use reactive co-sputtering and subsequent ammonia annealing to introduce Zr into Ta<sub>3</sub>N<sub>5</sub>, with the aim of investigating how the ternary nitride character of Zr-Ta-N(O) enables tuning of key semiconductor properties. Using a range of complementary characterization methods, we show that synthesis parameters and Zr content have a significant influence on the crystal structure, morphology, and optoelectronic properties of this ternary compound. Based on these insights, we optimize the composition and synthesis processes to achieve a highly stable and efficient photoanode material, which is a key requirement for solar water splitting.

KFM 21.8 Wed 17:15 H36

**Defect-Engineered Atomic Layer Deposited TaO<sub>x</sub> Protection Layers for Photoelectrochemistry** — ●TIM RIETH, CLARA SCHERM, and IAN SHARP — Walter Schottky Institute and Physics Department, Technical University of Munich, Am Coulombwall 4, 85748 Garching, Germany

Photoelectrochemical (PEC) energy conversion provides a viable route to the generation of chemical fuels from solar light. In this approach, charge carriers generated within a semiconductor light absorber immersed in an electrolyte are used to drive water splitting or carbon dioxide reduction reactions. A particularly relevant PEC configuration uses photovoltaic absorbers coated with transparent and conductive protection layers that prevent chemical corrosion of the semiconductor components. However, ensuring that the protection layer simultaneously fulfills the criteria for chemical stability, electronic conductivity, and optical transparency remains a challenging task. Here, we utilize plasma enhanced atomic layer deposition (PE-ALD) to create defect engineered and ultra-thin tantalum oxide (TaO<sub>x</sub>) protection layers for PEC applications. In addition to their optical transparency, the TaO<sub>x</sub> films form continuous coatings on the photoabsorber and provide improved chemical stability compared to titanium dioxide. A sufficiently high film conductivity is obtained by intentionally introducing electronic defects from hydrogen plasma sub-cycles during the ALD process. The demonstrated defect engineering mechanism and achieved TaO<sub>x</sub> protection layers represent an advance towards efficient and stable PEC devices.

KFM 21.9 Wed 17:30 H36

**Exploring novel ternary nitride semiconductor photoabsorbers for solar energy conversion applications** — ●LAURA I. WAGNER<sup>1</sup>, ELISE SIROTTI<sup>1</sup>, JOHANNA EICHHORN<sup>1</sup>, CHANG-MING JIANG<sup>1</sup>, MATTHIAS KUHL<sup>1</sup>, VERENA STREIBEL<sup>1</sup>, DAVID EGGER<sup>2</sup>, and IAN D. SHARP<sup>1</sup> — <sup>1</sup>Walter schottky Institut und TUM, München, Germany — <sup>2</sup>TUM, München, Germany

Solar water splitting offers the possibility to harvest the sunlight and store it in the chemical bonds of hydrogen. Exploratory research has revealed several possible photoanode materials, but until now no material meets the core requirements for photochemical stability, carrier extraction efficiency, and moderate band gap in the visible range. In this context, transition metal nitride semiconductors are underexplored and offer promise as new photoanode materials candidates. As a non-equilibrium synthesis approach, reactive magnetron co-sputtering enables the synthesis of novel ternary nitride photoabsorbers. In this work, a new ternary metal nitride photoanode material, cubic bixbyite-type ZrTa<sub>3</sub>N<sub>3</sub>, is presented. We observe the reactively sputtered Zr-Ta<sub>3</sub>N<sub>3</sub> thin films to exhibit an optical bandgap at 2.4 eV and n-type behavior. Most importantly, the resulting polycrystalline films exhibit appreciable photoactivity when implemented as a photoanode in a photoelectrochemical cell. Benefiting from the tunability of cation (Ta,Zr) ratio of reactive sputtering and anion (N,O) ratio with post annealing treatments, the solid solution of Zr<sub>x</sub>Ta<sub>2-x</sub>N<sub>3</sub>(O) offers a large param-

eter space to tune and optimize optoelectronic properties for various applications, including for PEC applications.

KFM 21.10 Wed 17:45 H36

**Electrical transport across catalyst/defect-engineered titania corrosion protection layer interfaces for light-driven CO<sub>2</sub> reduction** — ●JULIUS KÜHNE, OLIVER BIENEK, TIM RIETH, and IAN D. SHARP — Walter Schottky Institute and Physics Department, Technical University of Munich, Am Coulombwall 4, 85748 Garching, Germany

Producing value-added products via light-driven CO<sub>2</sub> reduction represents a promising approach to sustainably address increasing CO<sub>2</sub> emissions and meet the growing global energy demand. However, such solar fuels systems require passivating layers to chemically protect semiconductor light absorbers from harsh reaction environments. Despite great progress in the development of atomic layer deposited (ALD) protection layers, the factors governing efficient charge injection into the catalytic component are not yet well understood. Here, the charge transport characteristics between various defect-engineered TiO<sub>2</sub> protection layers grown with ALD and metal catalyst layers including Ag, Au, Pt, Ni and Ti are analyzed. This work aims to get a deeper understanding of the interface between catalyst and protection layer in terms of contact resistivity, carrier transport, and interface kinetics. Additionally, results of EC and PEC measurements are compared to assess the stability and activity of these systems under CO<sub>2</sub> reduction conditions in a two-compartment cell with ion exchange membrane. The selectivity of selected catalyst layers is evaluated by gas chromatography of the reaction products, thereby enabling a quantification of their overall performance characteristics.

KFM 21.11 Wed 18:00 H36

**Finite supercell charge correction for electronic transitions in defects including electronic and ionic screening** — ●CHRISTOPH FREYSOLDT<sup>1</sup>, BAOWING DOU<sup>1</sup>, STEFANO FALLETTA<sup>2</sup>, and JÖRG NEUGEBAUER<sup>1</sup> — <sup>1</sup>Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf — <sup>2</sup>Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

Charged point defects play an important role in the function of (opto)electronic devices. Theoretical investigations have proven valuable to understand quantitatively their stability, electrical and optical properties, and hence their beneficial or detrimental role in device performance. Electronic transitions involving localized defect states have recently moved into the focus. Similar to formation energies, also the transition energies suffer from artifacts due the long-range Coulomb interactions and the artificial periodicity in supercell models of defects. While the initial charge state is subject to full electronic and ionic screening, the changes upon the transition are screened by electrons only. Yet, the required charge corrections cannot be derived by cleverly combining traditional corrections for formation energies of initial and final state. I will present an overview of how these artifacts can be understood and corrected for. I will show applications for vertical transitions and non-radiative carrier capture.

KFM 21.12 Wed 18:15 H36

**Influence of Sr concentration on atomic, magnetic, and electronic structure of Ruddlesden-Popper oxide La<sub>2-x</sub>Sr<sub>x</sub>Co<sub>1-y</sub>Fe<sub>y</sub>O<sub>4</sub>** — ●DINA I. MAZITOVA<sup>1</sup>, DEBALAYA SARKER<sup>1,2</sup>, and SERGEY V. LEVCHEV<sup>1</sup> — <sup>1</sup>Moscow, Russia — <sup>2</sup>UGC-DAE CSR, Indore, India

Ruddlesden-Popper oxides were demonstrated to be promising catalysts for oxygen evolution reaction. There are numerous attempts in the literature to find descriptors for predicting a catalytic activity. However, the descriptors may depend on the distribution of ions of different types in these multi-component systems.

We calculated atomic, electronic, and magnetic structure of La<sub>2</sub>Co<sub>0.5</sub>Fe<sub>0.5</sub>O<sub>4</sub>, LaSrCo<sub>0.5</sub>Fe<sub>0.5</sub>O<sub>4</sub> (LSCFO), and Sr<sub>2</sub>Co<sub>0.5</sub>Fe<sub>0.5</sub>O<sub>4</sub> for different distributions of iron and cobalt using all-electron DFT in GGA and GGA+*U* approximations. Our calculations show that the favorable distribution of transition metal cations depends on the amount of Sr substituted in the A site. The electronic and magnetic structures depend strongly on the Fe/Co distribution. For example, GGA-RPBE calculations in LSCFO showed charge-ordered ferromagnetic structure in the Co layer and antiferromagnetic structure in the Fe layer when Co and Fe layers interchange with one another, but for uniform distribution of iron and cobalt ions, LSCFO becomes ferromagnetic.