

HL 38: Functional semiconductors for renewable energy solutions I

Time: Thursday 9:30–11:45

Location: POT 6

HL 38.1 Thu 9:30 POT 6

Energy landscape of B–Si defects calculated by DFT for modelling light-induced degradation in silicon — ●AARON FLÖTOTTO¹, WICHARD J.D. BEENKEN¹, KEVIN LAUER^{1,2}, and ERICH RUNGE¹ — ¹Technische Universität Ilmenau, Institut für Physik, Ilmenau, Germany — ²CiS Forschungsinstitut für Mikrosensorik GmbH, Erfurt, Germany

Boron is a technologically highly relevant p-dopant of silicon. Often, boron does not simply replace a silicon atom, but forms a B–Si pair that shares one lattice site. Several metastable pair configurations exist, with boron being closer to either a more substitutional or a more interstitial position. Using DFT, we calculated all neutral and charged metastable configurations of these defects and – using the Nudged Elastic Band algorithm – the minimal-energy paths between them. The resulting energy minima, barrier heights, and conversion rates will be discussed within the $A_{Si}-Si_i$ model for light-induced degradation (LiD) as suggested by K. Lauer et al. [1].

[1] for a recent review, see: K. Lauer, K. Peh, D. Schulze, T. Ortlepp, E. Runge, and S. Krischok, "The $A_{Si}-Si_i$ Defect Model of Light-Induced Degradation (LiD) in Silicon", *phys. status solidi A* 219, 2200099 (2022), <https://doi.org/10.1002/pssa.202200099>

HL 38.2 Thu 9:45 POT 6

Nanoscale characterization for understanding performance limitations in water splitting photoelectrodes — LUKAS WOLZ¹, HARISHANKAR BALAKRISHNAN², GUANDA ZHOU¹, IAN SHARP¹, ACHIM HARTSCHUH², and ●JOHANNA EICHHORN¹ — ¹Walter Schottky Institute, TU München, Am Coulombwall 4, 85748 Garching, Germany — ²Department of Chemistry, LMU München, Butenandtstr. 5-13, 81377 Munich, Germany

Economically viable systems for photoelectrochemical water splitting are often based of polycrystalline or nanostructured semiconductor thin films. Their nano- to micrometer properties often control critical processes, such as efficiency and stability, of the macroscale system.

Here, we aim at resolving local heterogeneities and at elucidating their effect on light-driven processes of $BiVO_4$ thin films using a correlative nanoscale approach. Scanning nearfield infrared microscopy shows varying absorption from VO_4 stretching modes across the film which correlates with local photoconductivity heterogeneities revealed by photoconductive atomic force microscopy. Furthermore, local temperature-dependent current-voltage spectroscopy in controlled gas environment shows that the low intrinsic bulk conductivity limits the electron transport [1], and that adsorbed oxygen acts as surface trap states for electrons [2]. Overall, combining insights from different nanoscale techniques generates a comprehensive picture of charge transport and transfer at the nanoscale, which provides the foundation for the rational design of durable and efficient solar fuel devices.

[1] *Nat. Commun.* 2597 (2018) [2] *ACS Interfaces*, 10, 35129 (2018)

HL 38.3 Thu 10:00 POT 6

Calibration of low temperature photoluminescence of boron doped silicon with increased temperature precision — ●KATHARINA PEH¹, AARON FLÖTOTTO¹, KEVIN LAUER^{1,2}, DIRK SCHULZE¹, and STEFAN KRISCHOK¹ — ¹TU Ilmenau, Institut für Physik und Institut für Mikro- und Nanotechnologien, 98693 Ilmenau, Germany — ²CiS Forschungsinstitut für Mikrosensorik GmbH, Konrad-Zuse-Str. 14, 99099 Erfurt, Germany

Low-temperature photoluminescence spectroscopy (LTPL) enables the determination of the dopant concentration of shallow impurities in silicon. We present a method which allows the determination of the boron concentration in silicon in a range from $10^{11} cm^{-3}$ to $10^{17} cm^{-3}$ at temperatures from 4.2 to 20 K with increased temperature accuracy. This method requires only one calibration function for the photoluminescence intensity ratio $I_{B_{TO(BE)}}/I_{I_{TO(FE)}}$. We obtain the measurement temperature from the intrinsic silicon photoluminescence line of free excitons ($I_{TO(FE)}$) using a fitting method, which distinguish the TO and LO components of the free exciton peak. The determined calibration function is $I_{B_{TO(BE)}}/I_{I_{TO(FE)}} = (5.8 \pm 0.08) \cdot 10^{-18} cm^3 \cdot c_{boron} \cdot e^{(56.7 \pm 0.7K)/T}$. The obtained exciton binding energy to boron, $E_b = 4.9 \pm 0.1 meV$, agrees well with literature data.

HL 38.4 Thu 10:15 POT 6

Coaxial Nanowire-in-Nanopore Arrays Enabling Anti-Agglomeration and Reliable Length Retention — ●CHENGZHAN YAN, HUAPING ZHAO, and YONG LEI — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany.

Nanowire arrays, a typical one-dimensional (1D) nanostructure used in energy storage systems, have significantly improved the electrochemical performance by optimizing the active material distribution and promoting the charge transport kinetics in energy storage systems. Notably, nanowire arrays with well-defined arrangements and high aspect ratios are of particular interest. To this end, one prevailing strategy is to combine ordered templates with wet chemical techniques. However, nanowires with high aspect ratios have a more severe tendency to agglomerate because of uneven capillary forces, which leads to poor arrangement reliability and degrades the electrochemical performance. Herein, the ultra-thin honeycomb alumina nanopores are constructed to ensure the structural stability of nanowire arrays, achieving a reliable quadrupling of the length. Based on the integrated nanowire-in-nanopore architecture, MnO_2 and polypyrrole are further electrodeposited on these free-standing nanowires to form vertically aligned core-shell 1D nanostructure arrays as cathodes and anodes for micro-supercapacitors (MSCs). Attributed to the high specific surface area and low charge diffusion resistance, these MSCs attain remarkably improved energy density, rate performance and lifespan.

30 min. break

HL 38.5 Thu 11:00 POT 6

Tails states, Voc loss and semiconductor compensation — ●SUSANNE SIEBENTRITT and OMAR RAMIREZ — University of Luxembourg, Laboratory for Photovoltaics

It has been shown for many solar cell absorbers that Voc loss correlates with the Urbach energy, which describes the decay of tail states into the band gap. In chalcopyrites it was furthermore observed that heavy alkali postdeposition treatments reduce both: Urbach energy and Voc loss. This behaviour has been attributed to passivation of grain boundaries. However, recently we have shown, that alkali treatment in single crystalline films without grain boundaries also leads to a reduction of Voc loss and Urbach energies. This behaviour can be traced back to a reduced compensation by increasing the doping level. It is to be expected that a similar mechanism plays a role in polycrystalline films. Part of the dependence of the Voc loss on Urbach energy can be attributed to radiative and non-radiative recombination in and through tail states. However, the dependence is stronger than would be expected from the increased recombination. We now understand that this is due to a simultaneous effect: increasing doping increases Voc and decreases tail states. Thus we propose, that one effect of heavy alkali treatment is due to the observed increase of Na doping inside the grains, because it increases the net-doping, reduces tail states and thereby reduces radiative and non-radiative recombination. All this increases Voc.

HL 38.6 Thu 11:15 POT 6

Dependence of the activation energy of light-induced degradation (LID) in silicon on the illumination intensity — ●KEVIN LAUER^{1,2}, KATHARINA PEH¹, DIRK SCHULZE¹, and STEFAN KRISCHOK¹ — ¹Technische Universität Ilmenau, Institut für Physik und Institut für Mikro- und Nanotechnologien, Ilmenau, Germany — ²CiS Forschungsinstitut für Mikrosensorik GmbH, Erfurt, Germany

It was found that the activation energy of the dissociation process of the acceptor-iron defects ($A_{Si}-Fe_i$) in silicon depends on the illumination intensity.[1] This implies that besides the thermal energy an additional supply of energy due to e.g. carrier recombination is possible in that defect reaction. To check whether this is also the case for the slow process of the light-induced degradation (LID) in silicon,[2] which can be explained by acceptor-silicon defects ($A_{Si}-Si_i$),[3] we measured the activation energy for the slow LID process for different illumination intensities. No impact of the illumination intensity on the activation energy of the slow LID process could be found indicating a pure thermally activated process.

[1] K. Lauer, C. Möller, D. Debbih, M. Auge, and D. Schulze, *Solid*

State Phenom. 242, 230 (2015).

[2] J. Lindroos and H. Savin, *Sol. Energy Mater. Sol. Cells* 147, 115 (2016).

[3] K. Lauer, K. Peh, D. Schulze, T. Ortlepp, E. Runge, and S. Krischok, *Phys. Status Solidi A* 219, 2200099 (2022).

HL 38.7 Thu 11:30 POT 6

Photoelectrochemical Catalyst Deposition on III-V Semiconductor Surfaces for Direct Solar Water Splitting — •ERICA SCHMITT, MORITZ KÖLBACH, MARGOT GUIDAT, MARCO FLIEG, MAX NUSSHÖR, ANNA-LENA RENZ, and MATTHIAS MAY — Universität Tübingen, Institute of Physical and Theoretical Chemistry, Tübingen, Germany

The conversion of solar electrical energy to chemical energy by the generation of hydrogen is believed to play a key role in the transition towards a sustainable energy system. One approach to generate

sustainable hydrogen is the use of III-V photoelectrodes in a highly efficient photoelectrochemical water splitting device. Such fully integrated, monolithic systems have a potentially lower balance of system cost compared to more conventional decoupled PV-electrolysis approaches and have already shown to be highly efficient [1].

The III-V semiconductor-electrolyte interface plays a crucial role in the performance of a photoelectrochemical device. Our work focuses on the photoelectrochemical modification of the semiconductor surface with a suitable catalyst and its stabilization in the harsh environment of an acidic electrolyte under operating conditions while also understanding the underlying physicochemical processes. We present an optimized functionalization process to increase the solar-to-hydrogen efficiency and stability of a photoelectrochemical cell, as well as the electrochemical and spectroscopical characterization using, among other methods, reflection anisotropy spectroscopy. [1] May, M., Lewerenz, H.J., Lackner, D. et al., *Nat. Commun.* 6, 8286 (2015).