



MARTIN-LUTHER-UNIVERSITÄT HALLE-WITTENBERG

Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany

OF SUR

Naturwissenschaftliche Fakultät II – Chemie, Physik und Mathematik

Dekan

Prof. Dr. Wolfgang H. Binder

Hausanschrift: von-Danckelmann-Platz 3 06120 Halle/Saale Germany

Tel.

+49(0)345 55-25501 +49(0)345 55-27158 dekan@natfak2.uni-halle.de

Fax

email Internet

www.natfak2.uni-halle.de

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Report of the Evaluation Committee of the "Zentrum für Innovationskompetenz SiLi-nano"

The following report covers the 2nd funding period (since 2016) of the ZIK SiLi-nano and was compiled by a Scientific Evaluation Committee. The committee based its findings on a comprehensive 90-pages activity report submitted by the ZIK SiLi-nano directors to the committee and the on-line meeting on 27. 11. 2020 as well as on personal discussions.

Members of the Scientific Evaluation Committee:

Prof. Dr. Wolfgang Binder (Chairperson)	Institute of Chemistry and Dean of Na- turwissenschaftliche Fakultät II	MLU Halle-Wittenberg
Prof. Dr. Stefan Ebbinghaus	Institute of Chemistry	MLU Halle-Wittenberg
Prof. Dr. Silke Christiansen	Institute of Optics, Information and Photonics	FAU Erlangen-Nürnberg
Prof. Dr. Kathrin Dörr	Institute of Physics	MLU Halle-Wittenberg
Prof. Dr. Radim Beránek	Institute of Electrochemistry	Ulm University

Brief timeline of ZIK SiLi-nano: The Center was founded at the start of the 1st BMBF funding period in 2009 with two research groups, "Silicon to Light" and "Light to Silicon". The group leader of "Silicon to Light", Prof. Jörg Schilling, became a full professor at the Institute of Physics in 2017. Dr. Paul Miclea, the leader of the other primary group, is a permanent scientist at the Fraunhofer Center for Silicon Photovoltaics (CSP). In 2016, two new groups were established after successful application for the 2nd BMBF funding period: "Light for High-Voltage Photovoltaics" and "Light for Hydrogen", led by Dr. Akash Bhatnagar and Dr. Wouter Maijenburg, respectively.

The evaluation meeting was organized as a video conference, because the Covid-19 pandemic regulations did not allow for a live meeting. The two junior group leaders appointed at the beginning of the

2nd funding period, Jun-Prof. Dr. Wouter Maijenburg (L4H group "Light for Hydrogen") and Dr. Akash Bhatnagar (L4HVPV group "Light for High-voltage photovoltaics"), gave 30 mins overview talks on the research of their groups, followed by discussion and feedback to the group leaders. In a subsequent poster session, 12 posters on scientific projects were video-presented by group members of all four groups of ZIK SiLi-nano. In a subsequent oral session, the group leaders from the 1st funding period, Prof. Dr. Jörg Schilling and Dr. Paul Miclea (groups "Light to Silicon" and "Silicon to Light"), introduced their work progress and received recommendations from the committee. The meeting closed with a final discussion about strategic directions of the ZIK and its research groups.

The overarching scope of research of the ZIK-SiLi-nano is the light-matter interaction in nanostructures for technologically relevant processes. Founded as a joint venture between the Martin-Luther-University Halle-Wittenberg (MLU), the Max-Planck-Institute for Microstructure Physics and the Fraunhofer Institute for Microstructure of Materials and Systems IMWS (in conjunction with the Fraunhofer Center for Silicon Photovoltaics CSP), the ZIK SiLi-nano maintains strong ties to these research institutions. Since 2010, the ZIK SiLi-nano has the status of an interdisciplinary scientific facility (IWE) at the Faculty of Natural Sciences II of the MLU. This status was extended for another 5 years in 2015 following its successful evaluation. A continuation for another 5-year period is now planned to extend the interdisciplinary concept of the ZIK SiLi-nano into the near and medium future. The ZIK groups successfully complemented their BMBF funding with three regular DFG projects and a EU project. A scanning electron microscope with electron-dispersive x-ray spectroscopy was co-funded by DFG and the county Sachsen-Anhalt in 2018 (Light for Hydrogen group). Further strong funding could be obtained from the Ministry of Research and Economy Sachsen-Anhalt.

2nd BMBF funding period: Jun-Prof. Dr. Wouter Maijenburg, Light for Hydrogen (L4H) Group

Scientific progress

Jun.-Prof. Maijenburg is associated with the Institute of Chemistry. The group presented 5 posters at the evaluation meeting. The L4H group has its research focus on quasi-one-dimensional nanostructures (like nanowires, nanotubes, nanofibers) for photoelectrochemical and electrochemical water splitting (hydrogen generation). Such 1D nanostructures offer large active surfaces and are particularly suitable for efficient photochemistry because of their similar light absorption depth and charge carrier diffusion length. The group has built an impressive portfolio of different kinds of nanostructures via wet-chemical methods, including metal organic framework (MOF) and metal oxide systems. They published 11 research papers in high and very high rank journals (like *Angewandte Chemie* and *Advanced Functional Materials*) which reflect an excellent scientific productivity, given the time span since 2016 and the teaching contributions.

Integration into the scientific landscape

The L4H group started working in October 2016 and, besides several own initiatives in setting up measurement facilities, uses equipment at the Institute of Chemistry. Jun-Prof. Wouter Maijenburg has a tenure option at the Institute of Chemistry after successful completion of the 2nd BMBF funding period. Since the winter semester 2016/2017, the L4H group is in charge of the course "Anorganische Chemie im Nebenfach (AC-NI)" which currently comprises of 2 SWS lectures and 4x 2 SWS seminars. Further lectures, seminars and practical courses have been covered by the L4H group since 2017 (as

detailed in the ZIK report booklet). In close collaboration with Prof. Ralf Wehrspohn (Institute of Physics) and the Max-Planck Institute for Microstructure Physics, an Oxford atomic layer deposition (ALD) system has been upgraded and adjusted for the specific research requirements. Joined research activities with Prof. Wehrspohn as well as with Prof. R. Scheer from the Institute of Physics are reflected in several publications.

Recommendations

The group has made very good progress in the synthesis of nanostructured, complex materials and, e.g., for the Cu-Ga-Se system high photocurrents have been measured. In the next step, more emphasis should be put on investigations of the actual water splitting reaction (i.e., evolution of H₂ and O₂), and possibly on (photo)electrocatalysis of further useful chemical transformations (e.g., selective conversions of low-value organic feedstock, CO₂, etc.). The research topics investigated by the group are very timely and address some of the key challenges of a future hydrogen economy. A continuation of the already successful research directions is therefore highly recommended.

2nd BMBF funding period: Dr. Akash Bhatnagar, Light for High-Voltage Photovoltaics (L4HVPV) Group

Scientific progress

The L4HVPV group undertakes research on the photovoltaic effect in ferroelectric and multiferroic materials. The so-called bulk photovoltaic effect in ferroelectric materials paves the way towards extremely high photovoltages (of the order of 50 V), far superior to those in semiconductors, while, on the other hand, photocurrents in oxide ferroelectrics are small. Major research activities of the group are focused on developing oxide thin film heterostructures, which produce large photovoltages. 5 PhD students belong to the group presently; four of them lively and convincingly presented their projects in the poster session. The group has an impressive publication record in relation to its short existence, with several regular articles in very highly ranked journals like Nature Communications and Advanced Materials.

Laboratory setup and integration into the scientific landscape

The group was established with primary funding from BMBF in 2016. Dr. Bhatnagar has set up a laboratory for thin film epitaxy with pulsed laser deposition (PLD) which his group uses for the growth of oxide heterostructures. Equipment for photoelectric measurements and force microscopy complement the created experimental basis appropriately. Dr. Bhatnagar has already developed strong collaborations to research partners at the MLU through participating as a project leader in a DFG-funded Collaborative Research Center (SFB 762 "Functionality of oxide interfaces"). This resulted in joint publications with the theory group of Prof. Ingrid Mertig, the experimental group of Prof. Kathrin Dörr (both at the Institute of Physics) as well as with the group of Prof. Stefan Ebbinghaus at the Institute of Chemistry. Microfabrication and electron microscopy tasks are carried out at the Interdisciplinary Center of Research (IZM). In agreement with his perspective as a group leader at the Fraunhofer CSP after completion of the 2nd BMBF funding phase, Dr. Bhatnagar has established ties to this institution (research on solar illumination test systems with Dr. Christian Hagendorf). Within the regional scientific landscape, the group cooperates with the Institute of Surface Engineering in Leipzig (Dr. Andriy Lotnyk), providing them with access to atomically resolved transmission electron microscopy (TEM) for

oxide nanostructures. In this way, Dr. Bhatnagar has built a solid experimental foundation for the research of his group. Additionally, he started collaborations with Indian, Korean and Spanish colleagues which strengthen his experimental opportunities and expertise in the field.

Recommendations

Given the impressive track record of Dr. Bhatnagar within the last few years, it is suggested to intensify the efforts to secure a permanent position for him at one of the research institutions in Halle.

1st BMBF funding period: Prof. Dr. Jörg Schilling, Silicon to Light Group and Prof. Dr. Paul Miclea, Light to Silicon Group

Scientific progress

The research in the Silicon to Light group focuses on the enhancement of light generation in silicon-compatible materials as well as on the investigation and enhancement of nonlinear optical processes in nanostructures. In the 2nd funding period, the investigated materials base broadened from originally silicon-centered to a flexible combination with other materials resulting in composite or hybrid nanophotonic devices. Key results have been obtained for revealing the impact of Mie resonators on Ge quantum dot luminescence and for hyperlenses based on Ag nanowire arrays. The group has been very productive in publishing and received substantial international visibility (reflected, e. g., in invited talks). The Light to Silicon Group is devoted to applied research in the field of femtosecond-laser micromachining of multilayers, in particular for photovoltaic elements and transparent conducting oxide (TCO) multilayers.

Integration into the scientific landscape

Prof. Jörg Schilling became full professor (W2 Professorship for "Nonlinear Nanophotonics") at the Institute of Physics in 2017. His group comprises of a senior researcher, a postdoc and 3 PhD students. Prof. Schilling teaches courses on Experimental physics for biology, food scientist and resource management students (3 SWS + tutorials) in winter and summer semesters and further courses detailed in the ZIK Report. Prof. Jörg Schilling and Prof. Miguel Marques (Theoret. Physics), together with colleagues from the Department of Informatics, developed the new BSc degree programme "Physik und Digitale Technologien (Physics and Digital Technologies)" which is a combination of a Physics degree with fundamental elements of Informatics. This course aims to qualify students for future tasks which require both a solid scientific knowledge and the ability to use computer sciences to solve timely challenges. The Silicon to Light Group has strong ties to the Institute of Physics (Prof. Schilling is the present director of the institute) which are reflected in several joined publications with Profs. R. Scheer, G. Schmidt and R. Wehrspohn. On national level, the group had a successful DFG project on silver nanowire hyperlenses with Prof. Carsten Reinhard (Laserzentrum Hannover/Hochschule Bremen). The work on Mie resonances with Dr. Mihail Petrov from ITMO (St. Petersburg) and Dr. Alexej Novikov from IPAM (Nishni Novgorod) was funded as a joint German-Russian DFG-RFBR project "Collective Mie-resonances for active elements in silicon photonics".

The group leader position of the "Light to Silicon" group was temporarily held by Dr. Dominiq Lausch before it was taken over by Dr. Paul Miclea in 2017. Dr. Miclea holds a permanent position at the Fraunhofer CSP. The group currently consists of a PhD student and a senior scientist, looking actively

to expand in the near future. Thus, the continuation of research in this group could be successfully secured with a new group leader, confirming the initial intention of an independent perpetuation of the ZIK groups after the initial funding period by the BMBF finishes.

Further points and recommendations

Within the last twelve years, the ZIK SiLi-nano has undoubtedly proven to be an excellent platform for young scientists to establish their independent research agenda and scientific career. It is suggested to investigate possibilities to keep this important and valuable role of ZIK SiLi-nano alive, for example by intensifying efforts to attract highly promising young scientists with external funding (ERC StG, Emmy Noether Programme, etc.) to join ZIK SiLi-nano and its infrastructure established within the past years. The incorporation of the new research topics on water splitting and high voltage photovoltaics was very successful and could open up new research perspectives for future coordinated research programmes in materials science in the faculty. In addition the interdisciplinary character of the ZIK SiLinano was clearly strengthened by establishing the two new groups with backgrounds in physics and chemistry. In this respect the ZIK SiLinano functions as an integrating structure in the faculty stimulating and facilitating the exchange of scientific ideas from different areas and subjects.

In conclusion the ZIK SiLi-nano has indeed flourished as an Interdisciplinary scientific facility (IWE). To continue this successful development of the ZIK an extension of the status as an IWE is strongly recommended.

Prof. Dr. Wolfgang Binder

(Chairperson of the Evaluation Committee)