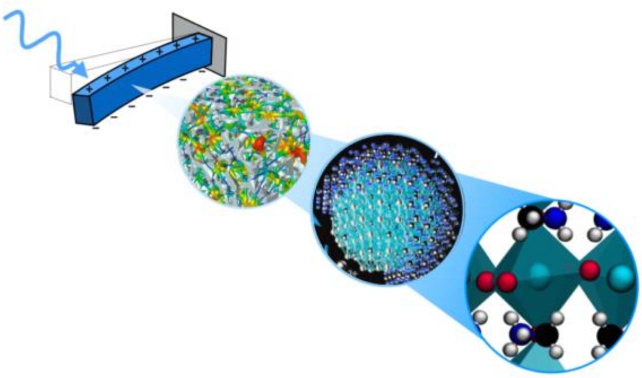
Annual Report 2020

of the International Research Training Group GRK 2495

in collaboration with Nagoya Institute of Technology (NITech)

Director: Prof. Dr. Kyle Webber

Co-Director: Prof. Dr. Ken-ichi Kakimoto



First funding period: 01.12.2020 – 30.06.2024

Impressum

Spokesperson:
Prof. Dr. Kyle G. Webber
Martensstr. 5, Room 1.43
91058 Erlangen
+49 9131 85-2754
kyle.g.webber@fau.de

Co-Spokespersom:
Prof. Dr. Ken-ichi Kakimoto
Frontier Research Institute for Material Science
Dep. Of Life Science and Applied Chemistry
Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan
kakimoto.kenichi@nitech.ac.jp

Coordinator:
Julia Berger
Martensstr. 5, Room 1.14
91058 Erlangen
+49 9131 85-27542
julia.b.berger@fau.de

Preface

Dear friends and colleagues,

The International Research and Training Group (IRTG2495) has been built upon the close collaboration and strategic partnership between FAU and NITech developed over the past decade, which originally started in the Materials Science and Engineering Department and in a short-time expanded to a University-wide connection. The IRTG, which started officially on January 1, 2020, represents an important next step in this partnership, which facilitates increased academic exchange as well as ever improved cultural understanding between Germany and Japan. Importantly, these activities are planned across numerous levels, integrating international experts from Japan into the FAU and German experts into NITech, both in terms of research as well as teaching and academic advising.

The primary focus of this joint project is the improved understanding of lead-free perovskite materials for electromechanical and photovoltaic energy conversion systems, where interdisciplinary research ranges from atomistic and continuum modelling, to materials development, to device integration. Development of lead-free systems is important due to increasing international regulations banning the use of heavy metals in, e.g., electronic devices. Such alternative energy sources will become increasingly vital over the next decades, not only as sources of renewable energy but also for high-tech applications, such as powering unattended wireless sensors. Of particular importance is the improved understanding of multi-length scale phenomena responsible for the energy conversion, development, and implementation of state-of-the-art lead-free perovskite materials, novel 2D and 3D processing techniques, and integration into devices. Various synthesis, manufacturing, and experimental techniques will be utilized and coupled to cutting edge simulations, facilitating interdisciplinary collaboration.

Of course, as in nearly every aspect of our lives, the ongoing pandemic has significantly changed our plans. This project, in particular, has been especially impacted due to the international nature and planned scientific exchanges, which have been and continue to be halted by travel restrictions. Despite these challenges, however, we have adjusted our ongoing activities to account for the ever-evolving situation, where we have developed new online international lecture series, graduate courses, training sessions, “hands-on” workshops, and even cultural exchange through care packages. As with everything, it is not the situation that defines you, rather how you respond to it. In this sense, the pandemic has really shown the adaptability of both the researchers in the IRTG as well as the strong collaboration between FAU and NITech.

Prof. Dr. Kyle Webber

At Nagoya Institute of Technology (NITech), our internationalization motto is focused on "developing global human resources who contribute to society". As an important practical example for that, our international training group has also been supported as a Japan-Germany Graduate Externship by the Japan Society for the Promotion of Science (JSPS). This joint project aims to establish international and interdisciplinary education research platform through active collaborative research between Japan and Germany, by sharing cutting-edge educational research facilities and providing interdisciplinary learning opportunities.

I think that the success of the project requires a deep, sharp and high-level research capability in the specialized field as the research element, and at the same time, interdisciplinary research collaborations through mutual access to diverse expertise beyond the boundaries of the fields. The innovative ideas from young researchers and students will become also a key to the success of this project.

Furthermore, through collaborative research projects, research not limited to one elemental technology available at one laboratory can be realized, and by forecasting its systematization, high value-added "idea of Monozukuri (Innovation)" can be acquired. In this sense, NITech strongly hopes to foster a solid partnership with FAU, so that we can continue to support each other.

Prof. Dr. Ken-ichi Kakimoto

Content

1. General Information

1.1. Participating Researchers

Principal Investigators (PIs)	Chair, Department, Address	Tel/ Fax, Email, Web	Research Area
Brabec, Christoph J., Prof. Dr.	Materials for Electronics and Energy Technology, Dep. of Materials Science and Engineering, Martensstr. 7, 91058 Erlangen	+49 9131 85-25426/-28495, christoph.brabec@fau.de, http://www.i-meet.ww.fau.de/	Semiconductors and Energy Devices
Cicconi, Maria Rita, Dr.	Glass and Ceramics, Dep. of Materials Science and Engineering, Martensstr. 5, 91058 Erlangen	+49 9131 85-27567/-28311, maria.rita.cicconi@fau.de, https://www.glass-ceramics.tf.fau.de/	Glass, Disordered Systems
Fey, Tobias, Dr.-Ing.	Glass and Ceramics. Dep of Materials Science and Engineering, Martensstr. 5, 91058 Erlangen	+49 9131 85-27546/-28311, tobias.fey@fau.de, https://www.glass-ceramics.tf.fau.de/	Cellular Ceramics
Fischer, Georg, Prof. Dr.-Ing.	Electronics Engineering, Dep. of Electrical, Electronical, and Communication Engineering, Cauerstr. 9, 91058 Erlangen	+49 9131 85-27186/-28730, georg.fischer@fau.de, https://www.lte.tf.fau.de/	Electronics for Communication
Heiss, Wolfgang, Prof. Dr.	Materials for Electronics and Energy Technology, Dep. of Materials Science and Engineering, Fürther Str. 250, 90429 Nürnberg	+49 911 56854-9216/-9351 wolfgang.heiss@fau.de, http://www.i-meet.ww.fau.de	Processing of Semiconductor Materials
Mergheim, Julia, APL Prof., Dr.-Ing.	Chair of Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen	+49 9131 85-28505/-28503, julia.mergheim@fau.de, https://www.ltm.tf.fau.de/	Computational Mechanics
Meyer, Bernd, Prof. Dr.	Computer Chemistry Center. Dep. of Chemistry and Pharmacy, Nägelsbachstr. 25, 91052 Erlangen	+49 9131 85-20403/-20404, bernd.meyer@fau.de, https://chemistry.nat.fau.eu/	Molecular Dynamics
Steinmann, Paul, Prof. Dr.-Ing.	Chair of Applied Mechanics, Dep.of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen	+49 9131 85-28501/-28503, paul.steinmann@fau.de https://www.ltm.tf.fau.de/	Continuum Mechanics
Webber, Kyle G., Prof. Dr.	Glass and Ceramics, Dep. of Materials Science and Engineering, Martensstr. 5, 91058 Erlangen	+49 9131 85-27551/-28311, kyle.g.webber@fau.de, https://www.glass-ceramics.tf.fau.de/	Functional Ceramics
Wellmann, Peter, Prof. Dr.-Ing.	Materials for Electronics and Energy Technology, Dep. of Materials Science and Engineering, Martensstr. 7, 91058 Erlangen	+49 9131 85-27635/-28495, peter.wellmann@fau.de, http://crystals.techfak.fau.de/	Crystal Growth
Wendler, Frank, Dr.	Materials Simulation, Dep. of Materials Science and Engineering, Dr.-Mack-Str. 77, 90762 Fürth	+49 911 65078-65067/-65066, frank.wendler@fau.de, http://www.matsim.techfak.uni-erlangen.de/	Phase Field Modeling
Zaiser, Michael, Prof. Dr.	Materials Simulation, Dep. of Materials Science and Engineering, Dr.-Mack-Str. 77, 90762 Fürth	+49 911 65078–65060/-65066, michael.zaiser@fau.de, http://www.matsim.techfak.uni-erlangen.de/	Statistical Multiscale Modeling

Haneda, Masaaki Prof. Dr.	Advanced Ceramics Research Center, Dep. Of Life Science and Applied Chemistry, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan	+81 52735-9964 Haneda.masaaki@nitech.ac.jp,	Heterogeneous Catalysts
Hayakawa, Tomokatsu, Prof. Dr.	Frontier Research Institute for Material Science, Dep. Of Life Science and Applied Chemistry, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan	+81 52735-5581 hayatomo@nitech.ac.jp	Optical Materials
Hayashi, Koichi, Prof. Dr.	Frontier Research Institute for Material Science, Dep. Of Physical Science and Engineering, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan	+81 52735-5308 Hayashi.koichi@nitech.ac.jp	X-ray characterization
Hirata, Akimasa, Prof. Dr.	Dep. Of Electrical and Mechanical Engineering, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan	+81-52735-7916 ahirata@nitech.ac.jp	Bioelectromagnetics
Kakimoto, Ken-ichi, Prof. Dr.	Frontier Research Institute for Material Science, Dep. Of Life Science and Applied Chemistry, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan	+81 00735-7734 Kakimoto.kenichi@nitech.ac.jp	Electronic Ceramics
Kato, Masashi, Prof. Dr.	Frontier Research Institute for Material Science, Dep. Of Life Science and Applied Chemistry, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan	+81 52735-5581 kato.masashi@nitech.ac.jp	Characterization of Energy Conversion Materials
Kawasaki, Shinji, Prof. Dr.	Dep. Of Life Science and Applied Chemistry, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan	+81 52735-5221 Kawasaki.shinji@nitech.ac.jp	Nanocarbon chemistry
Kosaka, Takashi, Prof. Dr.	Dep. Of Electrical and Mechanical Engineering, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan	+81 52735-5420 kosaka@nitech.ac.jp	Electric Machinery
Miyagawa, Reina, Prof. Dr.	Dep. Of Physical Science and Engineering, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan	+81 52735-5449 miyagawa.reina@nitech.ac.jp	Laser processing, Semiconductor
Ogata, Shuji, Prof. Dr.	Graduate School of Engineering, Dep. Of Physical Science and Engineering, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan	+81 52735-5372 ogata@nitech.ac.jp	Multiscale computer simulation of materials
Wang, Jianqing, Prof. Dr.	Dep. Of Electrical and Mechanical Engineering, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan	+81 52735-5457, wang@nitech.ac.jp	Wearable Communication Devices

Table 1: Participating Principal Investigators

Doctoral Resear-chers	Chair, Department, Address	Tel/ Fax, Email, Web	Research Area
Dobesh, David Kotato	Glass and Ceramics, Dep. of Materials Science and Engineering, Martensstr. 5, 91058 Erlangen	+49 9131 85-27556/-28311, david.dobesh@fau.de, https://www.glass-ceramics.tf.fau.de/	Glass
Gadel-mawla, Ahmed	Glass and Ceramics, Dep. of Materials Science and Engineering, Martensstr. 5, 91058 Erlangen	+49 9131 85-27558/-28311, ahmed.gadelmawla@fau.de, https://www.glass-ceramics.tf.fau.de/	Functional Ceramics
Gogoi, Niharika	Electronics Engineering, Dep. of Electrical, Electronical, and Communication Engineering, Cauerstr. 9, 91058 Erlangen	+49 9131 85-27188/-28730, niharika.gogoi@fau.de, http://www.lfte.de/	Electronic circuit design for energy harvesting
Freund, Tim	Materials for Electronics and Energy Technology, Dep. of Materials Science and Engineering, Martensstr. 7, 91058 Erlangen	+49 9131 85-27719/-28495, tim.freund@fau.de, https://www.i-meet.ww.uni-erlangen.de/	Crystal Growth
Hegendör-fer, Andreas	Chair of Applied Mechanics, Dep.of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen	+49 9131 85-64414/-64413, andi.hegendoerfer@fau.de, https://www.ltm.tf.fau.de/	Computational Mechanics
Köllner, David	Glass and Ceramics, Dep. of Materials Science and Engineering, Martensstr. 5, 91058 Erlangen	+49 9131 85-27549/-28311, david.koellner@fau.de, https://www.glass-ceramics.tf.fau.de/	Cellular Ceramics and Simulation
Kupfer, Christian	Materials for Electronics and Energy Technology, Dep. of Materials Science and Engineering, Martensstr. 7, 91058 Erlangen	+49 9131 85-27472/-28495, christian.kupfer@fau.de, https://www.i-meet.ww.uni-erlangen.de/	Semiconductors and Energy Devices
Maier, Juliana	Glass and Ceramics, Dep. of Materials Science and Engineering, Martensstr. 5, 91058 Erlangen	+49 9131 85-27557/-28311, juliana.maier@fau.de, https://www.glass-ceramics.tf.fau.de/	Functional Ceramics
Spreafico, Samuele	Computer Chemistry Center. Dep. of Chemistry and Pharmacy, Nägelsbachstr. 25, 91052 Erlangen	samuele.spr.spreafico@fau.de https://chemistry.nat.fau.eu/	Computational Chemistry
Stankie-wicz, Gabriel	Chair of Applied Mechanics, Dep.of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen	+49 9131 85-64411/-64413, gabriel.stankiewicz@fau.de, https://www.ltm.tf.fau.de/	Continuum Mechanics
Rehm, Viktor	Materials for Electronics and Energy Technology, Dep. of Materials Science and Engineering, Fürther Str. 250, 90429 Nürnberg	+49 911 56854-9351, viktor.rehm@fau.de, https://www.i-meet.ww.uni-erlangen.de/	Solution-Processed-Semiconductor-Materials
Veluri, Sai Prasanna	Left the IRTG in November 2020		
Choi, Minuk	Frontier Research Institute for Material Science, Dep. Of Life Science and Applied Chemistry, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan	m.choi.607@nitech.jp	Inorganic Solid-state Chemistry
Duan, Xianyi	Dep. Of Electrical and Mechanical Engineering, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan	x.duan.505@nitech.jp	Bioelectro-magnetic, Electromagnetic

Haque, Md Ismail	Dep. Of Electrical and Mechanical Engineering, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan	ismaileeeruetpg@gmail.com	Human body communication
Lobo, Ntumba	Dep. Of Electrical and Mechanical Engineering, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan	n.lobo.885@stn.nitech.ac.jp	Characterization of perovskite materials
Okada, Takeshi	Dep. Of Electrical and Mechanical Engineering, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan	t.okada.825@stn.nitech.ac.jp	Electric machines
Tsuzuki, Takahiro	Graduate School of Engineering, Dep. of Physical Science and Engineering, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan	t.tsuzuki.794@stn.nitech.ac.jp	Atomistic simulation of ferroelectric materials
Yamamoto, Yuta	Dep. Of Physical Science and Engineering, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan	y.yamamoto.276@stn.nitech.ac.jp	Atomic resolution Holography

Table 2: Participating Doctoral Researchers

Associated Researchers/ Post Docs	Chair, Department, Address	Tel/ Fax, Email, Web	Research Area
Biggemann, Jonas	Glass and Ceramics, Dep. of Materials Science and Engineering, Martensstr. 5, 91058 Erlangen	+49 9131-85 27561/-28311, jonas.biggemann@fau.de, http://www.glass-ceramics.uni-erlangen.de	Cellular Ceramics and Simulation
Dev, Chaitanya	Chair of Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen	+49 9131 85-64408/-64413, chaitanya.dev@fau.de, https://www.ltm.tf.fau.de/	Continuum Mechanics
Khansur, Neamul Hayet, Dr.	Glass and Ceramics, Dep. of Materials Science and Engineering, Martensstr. 5, 91058 Erlangen	+49 9131-85-2754/-28311, neamul.khansur@fau.de, http://www.glass-ceramics.uni-erlangen.de	Structure-property relationships in functional materials
Kirchner, Jens, Dr. Dr.	Electronics Engineering, Dep. of Electrical, Electronical, and Communication Engineering, Cauerstr. 9, 91058 Erlangen	+49 9131 85-27196/-28730, jens.kirchner@fau.de, http://www.lfte.de	Medical electronics and multiphysics systems
Mehnert, Markus	Chair of Applied Mechanics, Dep. of Mechanical Engineering, Egerlandstr. 5, 91058 Erlangen	+49 9131 85-67623/-28503, markus.mehnert@fau.de, https://www.ltm.tf.fau.de/	EAP
Osvet, Andres, Dr.	Materials for Electronics and Energy Technology, Dep. of Materials Science and Engineering, Martensstr. 7, 91058 Erlangen	+49 9131 85-27726/-28495 andres.osvet@fau.de, https://www.i-meet.ww.uni-erlangen.de/	Semiconductors and Light
Ritterhoff, Christian	Computer Chemistry Center. Dep. of Chemistry and Pharmacy, Nägelsbachstr. 25, 91052 Erlangen	christian.ritterhoff@fau.de https://chemistry.nat.fau.eu	Molecular Dynamics Simulations
Sytnyk, Mykhailo, Dr.	Materials for Electronics and Energy Technology, Dep. of Materials Science and Engineering, Fürther Str. 250, 90429 Nürnberg	+49 911 56854-9210/-9351 misha.Sytnyk@fau.de, https://www.i-meet.ww.uni-erlangen.de/	Optoelectronics
Martin, Alexander, Dr.	Dep. of Life Science and Applied Chemistry, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan	+81 52735-5588 martin.alexander@nitech.ac.jp	Electronic Ceramics

Table 3: Participating Associated Researchers and Post Docs

Students Assistants	Project, Supervisor	Research Area	Member (from – to)
Akca, Seda	Project E, Andres Osvet	Advanced Materials and Processes	Nov 2020
Emmel, Robin	Coordination, Julia Berger	Nanotechnology	Nov 2020
Eyoum, Gina	Project H, Kyle Webber	Functional Ceramics	May 2020
Halmheu, Melissa	Project F, David Köllner	Materials Science and Engineering	Oct.2020 – Dec 2020
Hanisch, Benedict	Project H, Kyle Webber	Nanotechnology	Jan 2020 – Feb 2020
Heyi, Zhang	Project E, Andres Osvet	Physics	Nov 2020
Hilpert, Felix	Project J, Wolfgang Heiss	Nanotechnology	Apr 2020
Hoffmann, Patrizia	Project D, Jonas Biggemann	Materials Science and Engineering	Jan 2020
Moorthy, Ventakesh Kumar	Project B, Paul Steinmann	Computational Engineering	Sep 2020 – Dec 2020
Mehta, Sharly	Project F, Juliane Maier	Chemical Engineering	Oct 2020
Nagaraj, Vinay	Project B, Gabriel Stankiewicz	Mechanical Engineering	Nov 2020
Novak, Jan	Coordination, Julia Berger	Materials Science	Nov 2020
Prakash, Vinay	Project B, Gabriel Stankiewicz	Computational Engineering	Apr 2020 – Jul 2020
Rohmer, Daniel	Project I, Peter Wellmann	Materials Science	Sep 2020
Schmidt, Bernd	Project L, Bernd Meyer	Chemistry	Apr 2020
Simon, Swantje	Project D, Jonas Biggemann	Material Science and Engineering	Jan 2020 – Dec 2020
Vo, Nadia	Project G, Rita Cicconi	Nanotechnology	Aug 2020
Zeair, Omar	Project H, Ahmed Gadelmawla	Chemical Engineering	Nov 2020

Table 4: Student Assistants

Industrial Advisors	Affiliation	Expertise
Picht, Gunnar, Dr.	Robert Bosch GmbH (Stuttgart)	Ferroelectrics, transducers for automobile applications
Schmidt, Oliver, Dr.	Siemens Healthineers , Technology, Innovation, Technology & Innovation Center, Basic Medical Technologies, (Erlangen)	Perovskite x-ray detectors
Fujii, Toru	TAIYO YUDEN Co.,Ltd.	Research and Development Laboratory, Dep.of Functional Device Development & Development Planning

Table 5: Industrial Advisors

Coordination and Administration	Work Address	Tel/ Fax, Email, Web	Work Area
Berger, Julia	Martensstr.5, 91058 Erlangen	+49 9131 85-27542/-28311, julia.b.berger@fau.de	Coordination and Administration
Shinkai, Taeko	Nagoya Institute of Technology	+81 52735-5019, shinkai.taeko@nitech.ac.jp	Assistant Administrative Staff

Table 6: Coordination

Group picture taken at the Kick-off Meeting

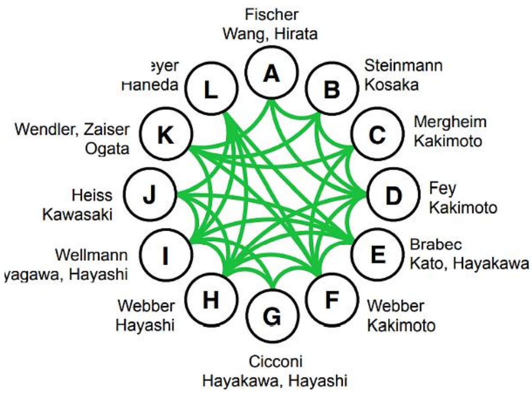
1.2. Reporting Period

01 January 2020 to 31 December 2020

2. Research Program

The aim of this IRTG is to create an international learning lab to train the next generation of scientists and engineers to work on sustainable energy, specifically electro-optical and electro-mechanical energy conversion systems based on lead-free perovskite-based materials. These complementary energy conversion techniques bring together two closely related fields to facilitate an interdisciplinary exchange, both at the FAU as well as internationally with NITech. Due to the nature of such systems, bringing together an interdisciplinary team of researchers that span the important length scales is vital, which allows critical, length-scale-specific phenomena to be directly addressed in a collaborative research and training environment. This resulted in a novel combination of research subjects. In addition, the enhanced internationalization provided by the IRTG facilitates international access to a wide array of experimental techniques and measurement equipment, extensive and varied expertise in atomic-scale to macroscale modeling, experimentation, and manufacturing techniques.

In order to achieve the training and research objectives, the IRTG is organized into twelve research projects that are specifically designed to be an interdisciplinary network that establishes nontraditional connections between research areas that may not be likely outside of such a framework, such as simulations and experimentation as well as electro-optical and electro-mechanical properties of the same material class.



Project Connections

First Meeting with doctoral researchers in January

A - Electronic Circuits for Piezoelectric Energy Harvesting and Sensor Array Systems

FAU: Niharika Gogoi, Georg Fischer and Jens Kirchner
NITech: Md Ismail Haque, Xianyi Duan, Jianqing Wang, Akimasa Hirata, Jose Gomez-Tame, Yinliang Diao, Junqing Lan and Anzai Daisuke

Objectives and status

The main objective of our project is to design an electronic circuit for multiport and asynchronous piezo energy harvesters, such that it can provide a regulated and stable usable output, in spite of the irregular nature of input excitations. A high conversion efficiency of the circuit is the primary goal in the circuit design. Along with the energy harvesting aspect, the project also focuses on the potential of piezo ceramics to be simultaneously used as sensors and energy harvesters. The sensory data is also useful for health care monitoring and sports training.

The project is currently divided into three sections that we are working on simultaneously:

- Electrical Modelling: Equivalent circuit model for the piezo ceramics to relate mechanical measures to the electrical output
- Human Gait Acquisition Circuit: An array of piezo ceramics are placed on a shoe inlay and human gait acquisition circuit is developed
- Electronic Circuitry: Comparative study of three different types of rectifier circuits

Conclusions, main achievements and outlook

1. Electrical Modelling: An electrical equivalent model expresses the electrical behavior of the ceramics in terms of electric circuit components and thus allows integrating the piezo into circuit simulations. We take two approaches to derive such a model. Firstly, we design an electrical model by impedance analysis and secondly we derive the model via Finite element analysis. Secondly, in association with Project C, we aim to relate the mechanical to the electrical parameters for a transducer model.

Achievement: The figure below shows an easy model to represent piezo ceramics by an electrical equivalent circuit. The model is based on the second approach.

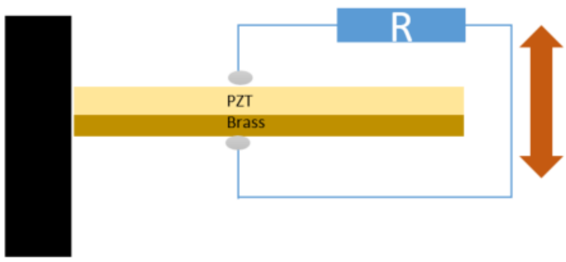


Figure 1 FE model for which the electrical model is derived.

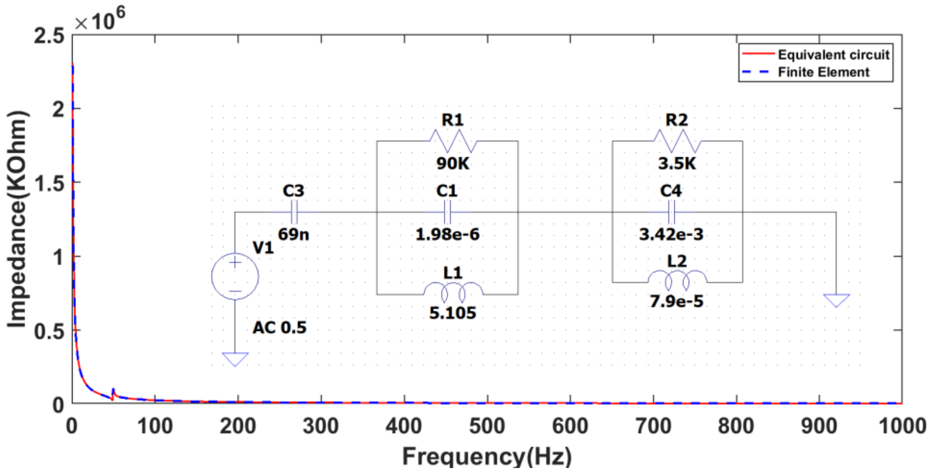


Figure 2 Easy model of electrical equivalent circuit of piezo ceramics

2. Human Gait Acquisition Circuit: The generated energy is expected to correlate with the gait pattern. Therefore, we design a human gait acquisition circuit is to assess the gait pattern of the foot movement. To this end, we integrate multiple piezo ceramics on a shoe inlay and acquire the sensory data.

Achievement: Layout design, ordered components. In addition, we are working in integration of components in the layout.

3. Electronic Circuitry: The electronic circuitry is responsible to convert the uncertain energy generation into constant supply of power output. To choose the appropriate circuitry, we made a comparative study of three different types of rectifiers for different types of input waveforms. This work involves both simulation and hardware approach. We have only done the simulations using an electrical equivalent circuit. The hardware task will be accomplished by triggering a commercial piezo disc.

Achievement: Active rectifiers shows the best results in simulations

The research idea was inspired from a smart shoe design. The fundamental point of our research idea is that walking/running activity would stimulate energy generation and sensing to predict human gait pattern. The energy generation significantly depends on the plantar anatomy, weight of the person and frequency of the activity. Therefore, every individual would deliver different levels of energy. On the other hand, the gait pattern would offer suitable applications in medical diagnosis, health monitoring and sports training.

We proceed with our research by taking into consideration the challenges and inconsistency in this area. As a starting point, we start our experiment with easily available lead contained piezo ceramics. Later on, we optimize our research with the lead free perovskite ceramics.

We have collaborated with projects C, F and H for our research. We associate with project C for electrical modelling of the piezo ceramics. The association with projects F and H was pursued to deploy their lead free Perovskite ceramics in our project. Furthermore, there is a collaborative project with Project B and G on the topic of electro-mechanical and electro-optical coupling. My role in this project is contributing in rectification of electrical signals.

“Can piezoelectric energy power an antenna integration beacon?”- This is the question the two sub groups of Project A wants to address. The NITech group aims to navigate elderly by mounting antennas on shoe sole. In collaboration with FAU, we are interested to investigate if the power generated from piezo-based shoe sole will be sufficient to power the antenna integration beacon.

B - Excitation-Conforming, Shape-Adaptive Mechano-Electrical Energy Conversion

FAU: Paul Steinmann, Gabriel Stankiewicz and Chaitanya Dev
NITech: Takashi Kosaka, Takeshi Okada and Yoshiki Sakuma

Objectives and status

Automobile manufacturers have been promoting electrification by introducing vehicles with electric drive systems such as hybrid electric, battery electric, and fuel cell vehicles to reduce CO_2 emissions. In order to further spread such low energy consumption vehicles, demands for high performance traction motors are growing. In addition to the motor efficiency and power density improvements, since vibration and noise transmitting from the motor to the vehicle body frame prevent from realizing the comfort in interior living space as well as are unfavorable to the outside of the vehicle, it is indispensable to reduce them. Therefore, we have been working on the research concerning with the reduction of vibration and noise generated from the electric motor using a dynamic vibration absorber (DVA) based on "Compliant mechanism". The compliant mechanism has an integral structure and can achieve functions similar to an ordinary mechanism by giving flexibility to the appropriate part of its structure rather than joints. With its jointless structure, miniaturization and cost reduction by reducing the number of parts and high reliability owing to life time prolongation can be expected. In addition, a variable stiffness mechanism can be realized by adding an actuator to the DVA based on the compliant mechanism. It is aimed to realize the DVA which can control and suppress the multiple natural vibrations of the electric motor running various angular frequencies.
In this research up to now, we have worked on the finite element analysis- (FEA-) based modeling of the motor mechanical characteristics and the DVA design using topology optimization. By attaching the designed DVA to the motor, the suppression effect of the vibration near a natural frequency of the motor has been confirmed by FFA-based frequency response analysis.

Additionally, the algorithmic framework for shape optimization has been developed and implemented into a c++ software, which allows for a frequency tuning of cantilevered, bimorph energy harvesters. Development of a novel approach to couple topology and shape optimization is currently in progress and can be employed to simple, purely elastic benchmark problems.

Conclusions, main achievements and outlook

To make our study simple as the first step, we treated a partially cut stator model of our test motor and worked on the derivation of mechanical characteristics of the stator model and the DVA design based on topology optimization.

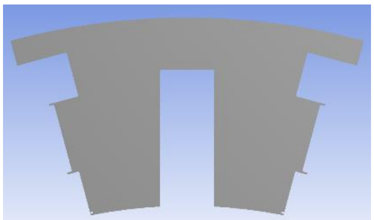


Figure 1 Sectional view of 1/12 stator partial model of target motor

Fig. 1 depicts the 1/12 partially cut stator model and Table I summarizes the results of mechanical characteristics derived, respectively. Fig. 2 illustrates the DVA designed based on the mechanical parameters of the target partial stator model, topology optimization and fixed-points theory[1]. Table I also includes the design results of DVA. The DVA shown in Fig. 2 is designed focusing on the 4th natural mode vibration of the target motor shown in Table I, and comprises a lead acting as a mass and a body composed of PA12 acting as a spring as well as supporting the mass. The lower part of body of DVA is attached to the outer periphery surface of stator of target motor to for absorbing the motor vibration. Fig. 3 shows FEA-computed results of the frequency responses of inertance of the motor without and with the DVA installed. From the figure, it can be seen that the 4^{th} mode natural vibration of target motor can be greatly reduced by applying the designed DVA. Specifically, the peak value of the inertance can be reduced by approximately 34%.

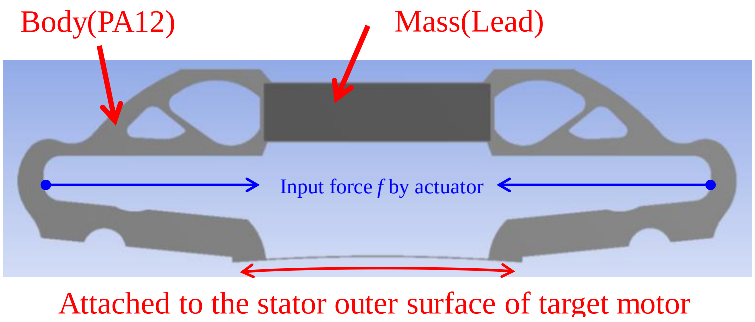


Figure 2 Designed DVA

[1] Brock, J. E., "A note on the damped vibration absorber," Journal of Applied Mechanics, Vol. 68, pp. A-284, 1946.

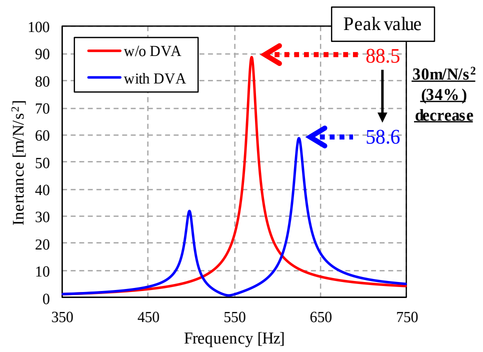


Figure 3 Frequency respons of the inertance with and w/o DVA installed

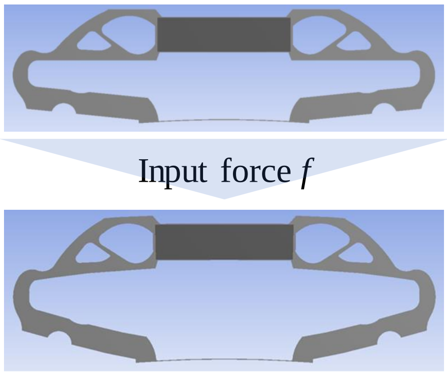


Figure 4 Shape change example of DVA operated by attached actuator.

As the next research step, we have started further investigation into DVA design. If a force is inputted to the designed DVA by an attached actuator as shown by blue arrows in Fig. 2, the DVA shape can be deformed as shown in Fig. 4. As a result, the natural frequency of the deformed DVA changes as appeared in Table II. However, as can be found from Tables I and II, it seems difficult to design the DVA that is capable of responding to all the natural frequencies of the motor widely varying with its operating angular frequency. As future works, therefore, we will continue to research the structure of the DVA that can work for suppressing all the natural frequencies of the motor, and how it is effective to change the sha pe by an attached actuator.

We have worked on the design of an object-oriented c++ software together with the IRTG associate researcher, M.Sc. Chaitanya Dev, which offers a ground structure for shape and topology optimization. The software is easily extendable, i.e. implementation of new optimization problems can be performed efficiently by making use of a shared functionality implemented for other optimization problems. The developed c++ software served as a starting point for the work towards optimization of energy harvesters. In order to fulfill the long-term goal to design the excitation-conforming, shape-adaptive energy harvesters, a number of steps has to be accomplished on the way. Up to date, an eigenvalue problem for cantilevered, bimorph energy harvesters was modeled and implemented. The equations for design sensitivity analysis with respect to the shape design of resonance and antiresonance eigenvalues in electroelastic problem were derived and implemented. After completing the previously mentioned tasks, frequency tuning of bimorph energy harvesters by shape optimization is possible. Verification of the optimized results for electric power output performance is done in cooperation with M.Sc. Andreas Hegendörfer from the Project C.

Table I Mechanical parameters of 1/12 partial stator model and DVA design results

Mass of stator [kg]	0.5651
Natural frequency of stator [Hz]	118.75 (2nd) 570.31 (4th) 928.13 (6th)
Modal mass of stator [kg]	1.9292 (2nd) 1.9311 (4th) 1.9307 (6th)
Modal stiffness of stator [kN/m]	$3.146*10^2$ (2nd) $7.252*10^3$ (4th) $1.921*10^4$ (6th)
Modal damping of stator [Ns/m]	8.432 (2nd) 40.47 (4th) 65.87 (6th)
DVA mass[g]	56.4
Natural frequency of DVA [Hz]	553.05

C - Macroscale Continuum Modeling and FE Simulation of Electromechanical Coupling in Perovskite-Based Materials

FAU: Julia Mergheim, Andreas Hegendörfer and Markus Mehnert
NITech: Ken-ichi Kakimoto

Objectives and status

A piezoelectric vibration-based energy harvester (PVEH) is composed of an electromechanical structure along with an energy extraction circuit. The objective of such a device is converting otherwise unused mechanical energy to electric energy to power e.g. wireless sensors. The piezoelectric effect, used as the energy conversion principle, describes the appearance of electrical voltage when the piezoelectric material is mechanically deformed and vice versa.

In some applications the electromechanical structure and the electric circuit have an influence on each other. This necessitates the accurate modeling of both parts and their interactions. The literature proposes different approaches for the simulation of such a combined device, e.g.:

- analytical modeling approaches[2], restricted to simple harvester geometries and linear models;
- equivalent circuit models[3], prohibiting the evaluation of mechanical variables in the electromechanical structure as strains or stresses;
- versatile Finite Element (FE) based approaches[4].

However, until now all FE based methods reported in literature, which are not coupled to a circuit simulation software, are limited to linear circuit elements and passive electrical interfaces. The FE based methods, which are combined with an external circuit simulation tool, consider only linear electromechanical structures or the coupling between the electromechanical structure simulation and the electric circuit simulation is not very efficient. To overcome the mentioned drawbacks of existing FE methods for PVEH the objective of the project is to develop a FE based approach, which can simulate nonlinear behavior of electromechanical structures as well as nonlinear and active electric circuits. Our method allows for consistent and efficient simulations of the complete possibly nonlinear PVEH using only one software tool.

Moreover, the developed FE code was utilized to compute the power output of shape optimized electromechanical structures in cooperation with project B. Furthermore, numerical simulations were carried out for project A, to provide data for an equivalent circuit model of a piezoceramic disk for an energy harvester mounted in a shoe. In cooperation with NITech, the properties of piezoceramic polymer-fiber composite materials were derived by means of numerical homogenization methods. Energy harvesters made of these composite materials were experimentally analysed at NITech and the data was utilized to validate the numerical simulations.

Conclusions, main achievements and outlook

The following milestones were reached:

- FE code for transient simulations of linear electromechanical structures.
- Simulation of nonlinear behavior of electromechanical structures.
- Parallelization of the FE code to allow for efficient computations.
- Automatic differentiation to easily adapt the FE code to different materials.
- Extension of the FE code by nonlinear or active electrical circuit elements.
- Validation of the developed FE method with results from literature.
- Simulation of an active power circuit coupled to a nonlinear electromechanical.

[2] Erturk A and Inman DJ A distributed parameter electromechanical model for cantilevered piezoelectric energy harvesters. *Journal of Vibration and Acoustics* 130(4): 041002.
[3] Elvin NG and Elvin AA (2009b) A general equivalent circuit model for piezoelectric generators. *Journal of Intelligent Material Systems and Structures* 20(1): 3-9.
[4] Gedeon D and Rupitsch SJ (2018) Finite element based system simulation for piezoelectric vibration energy harvesting devices. *Journal of Intelligent Material Systems and Structures* 29(7): 1333-1347.

- Publish the newly developed method and the results. Status: *In Progress*

Figure 1 presents the system simulation of a bimorph PVEH with a SSHI interface under base excitation. Considering nonlinear mechanical behavior of the electromechanical structure leads to a significant reduction of the harvested energy. Our approach allows to simulate the complete PVEH problem with a nonlinear and active electronic interface only using the finite element method. Hence, the structural simulation capabilities of the finite element method can be exploited.

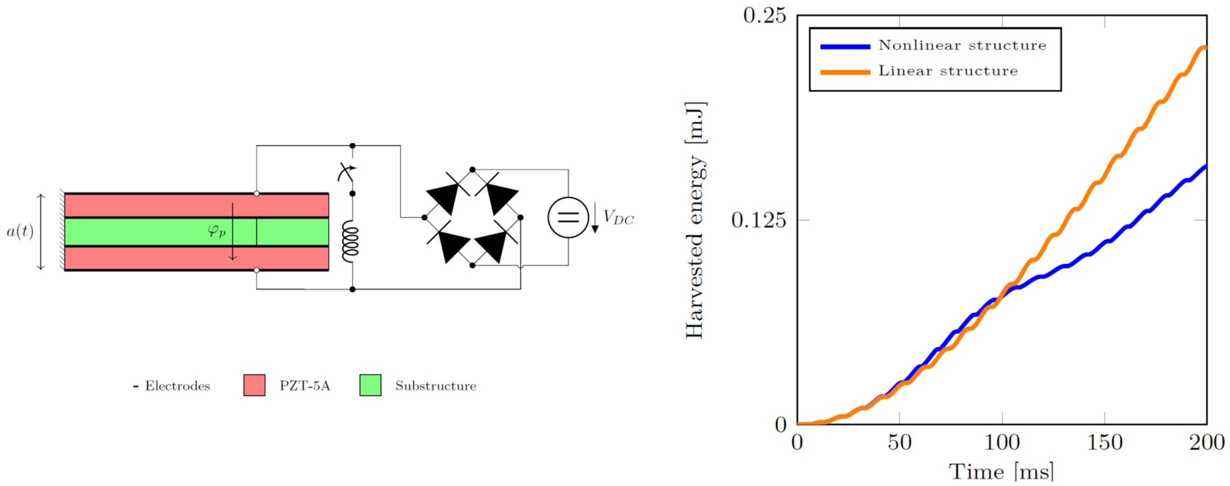


Figure 1: A base excited bimorph PVEH with a SSHI interface and the harvested energy when considering linear and nonlinear behavior of the electromechanical structure.

A future focus is on modeling and simulation of the hysteresis behavior of lead-free piezoceramics. The development of an electro-mechanically coupled nonlinear material model is to be carried out in close cooperation with Project H, which investigates the material behavior experimentally.

D - Additive Manufacturing of Cellular Lead-Free Ceramics

FAU: Tobias Fey, David Köllner and Jonas Biggemann
NITech: Ken-ichi Kakimoto

Objectives and status

The aim of this work is the fabrication and characterization of lead-free cellular ceramics. The focus is on the additive manufacturing of auxetic or auxetic-like structures to develop innovative lightweight and flexible sensor and energy harvesting systems. Another focus is the influence of design parameters, such as polarization direction, internal porosity, Poisson's ratio of the lattices, on the electromechanical properties. In the first year of the project, the main topic was mainly on the production and optimization of the building blocks regarding the processability of the starting materials, as well as basic properties such as porosity and piezoelectric properties, which has now been completed. In the next phase, internal porosity can be introduced in a targeted manner without other effects influencing this. A second important achievement is the establishment of an adapted process to fabricate complex cellular structures from monolithic ceramics, which was a core challenge. Monolithic lattices as well as building blocks form the basis for the characterization and the main goal of modular auxetic lattice structures.

Conclusions, main achievements and outlook

In the first section, the established injection molding process was used to produce ceramic building blocks from barium titanate and BCZT. For this purpose, the powders were first characterized in terms of particle size (1,5-3,5 µm) and specific surface area (1-2 m^2/g), as both are important parameters for the production of injection molding compounds. To produce the building blocks, a positive mold is first printed using stereolithography, which is then molded with silicone. The silicone mold is then filled with the ceramic injection molding compound and demolded after cooling. The ceramic green body is then debinded and sintered. After initial tests, the porosity of the building blocks was still between 10-20%, which greatly reduced the piezoelectric and mechanical properties. To reduce the porosity, three different injection molding compounds with solid contents between 50-59% were produced and the sintering temp. (1300-1500°C) and sintering time (3-6h) were varied. The optimized parameters reduced the porosity of BT to 4 ± 1.5% and BCZT to 2.3 ± 1.5%.

Because complex structures broke during the demolding of silicone molds, the process was modified to produce lattices. As shown in figure 1, the negative mold is first printed from water-soluble PVA via fused filament fabrication (FFF). This is in turn filled with the injection molding compound and the PVA is dissolved with distilled water. The production of different Lattice structures is one of the main achievements, because now it´s possible to examine the influence of structural parameters on the piezoelectric and mechanical properties. The focus here is on the Poisson's ratio, which can be varied by different parameters such as the angle and dimensions of the unit cells. Using a mathematical model, it has already been possible to produce transparent polymer lattices with a Poisson's ratio between -2 and 2 via stereolithography, on which photoelasticity is being measured in cooperation with project G. These measurements should help to optimize the structure for ceramic components in order to reduce stresses.

In cooperation with Project F, permittivity and piezoelectric measurements were carried out to investigate the material properties. In addition, measurements of the complex lattices are prepared. Cooperation with project B is also planned in order to optimize the auxetic structures through simulations.

The project has benefited from the cooperation with NITech, who are experts in the synthesis of BCZT. This powder was used in larger quantities to produce building blocks and lattice structures and could thus make a great contribution to the characterization.

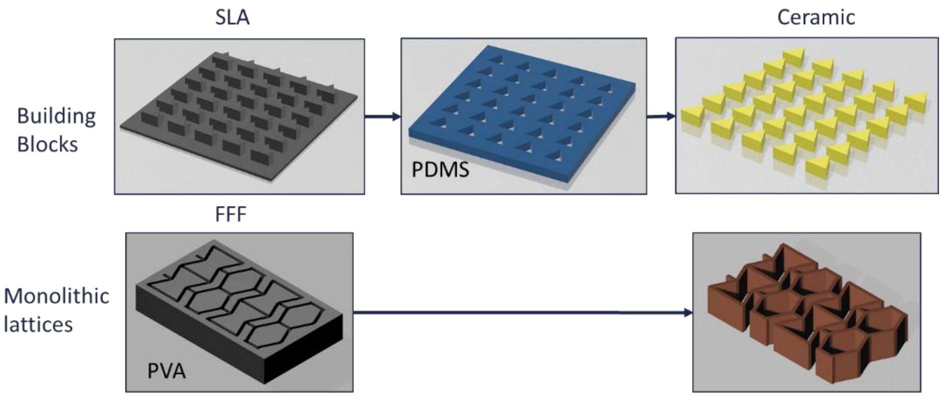


Figure 1.: Production steps for building blocks and monolithic lattice structures.

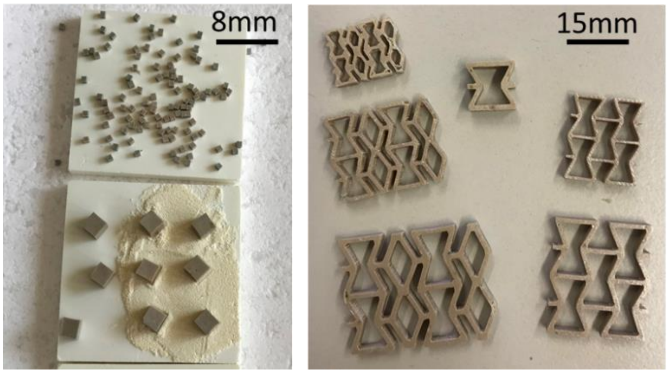


Figure 2.: Bariumtitanate building blocks and auxetic lattice structures with different size and poisson ratio.

E - Lead Free Perovskite Semiconductors with Tunable Bandgap for Energy Conversion

FAU: Christoph Brabec, Christian Kupfer and Andres Osvet
NITech: Tomokatsu Hayakawa, Masashi Kato, Ntumba Lobo and Min Uk Choi

Objectives and status

Prof. M. Kato's focus was on designing solar-to-hydrogen energy conversion with high efficiency using perovskite materials. For this, understanding of charge carrier dynamics is important. Therefore, charge carrier dynamics in perovskite materials were observed by photoluminescence and photoconductivity measurements. Moreover, Raman spectroscopy, performed under Prof. T. Hayakawa's supervision, is used to collect structural information of perovskite materials developed in this project.

The research performed by Christian Kupfer under the supervision of Dr. A. Osvet and Prof. C. J. Brabec aims to improve the understanding of perovskite semiconductors for solar cell applications. To achieve this, advancements in high-throughput characterization are pursued and a set of Cesium Titanium halides is synthesized and characterized.

Conclusions, main achievements and outlook

The group of Prof. M. Karo found, that when charge carriers are excited by light with short wavelength (266 nm), which is mainly absorbed near the material surface, carriers recombine faster compared to conventional long wavelength excitation with 355 nm. This indicates the significance of surface recombination of charge carriers.

In addition, in some materials, charge carriers were excited by light with sub-bandgap energy, and thus the energy levels exist within the band gap. These results suggest that control of surface and bulk defects is critical to maximize the energy conversion efficiency.

In the Raman investigation, performed under Prof. T. Hayakawa, vibrational modes ranging from several 100 to 2000 cm^{-1} were observed for $FAPbBr_3$ and $MAPbBr_3$ by near infrared laser excitation at 785 nm, which enabled deeper understanding of the structures of hybrid perovskite materials.

Mr. Kupfer successfully synthesized the vacancy-ordered double-perovskites Cs_2TiBr_6 and Cs_2TiI_6 using high-energy ball-milling. To the best of our knowledge, this is the first time these materials have been produced with a mechanochemical synthesis route. Additionally, a method and setup for quickly performing time-resolved photoluminescence measurements for charge carrier lifetime determination was employed. Furthermore, a microwave photoconductivity measurement setup was built, inspired by a similar setup from Prof. M. Kato's laboratory.

Prof. C. J. Brabec initiated and contributed to two European Research consortia on advanced solar cell technologies. Additionally, he is a member of two European INFRAIA consortia with the goal of building and integrating infrastructure on European scale. These consortia are open for all European researchers, from both academia and industry, ensuring their optimal use and joint development. One centre works on "printed organic electronics" while the other focuses on "perovskites".

F - Room Temperature Aerosol Deposition of Lead-Free Ferroelectric Films for Energy Conversion Systems

FAU: Kyle G. Webber, Juliana Maier, Neamul Hayet Khansur and Udo Eckstein
NITech: Ken-ichi Kakimoto and Alexander Martin

Objectives and status

The goal of the project is the deposition of lead-free ferroelectric thick films by room temperature aerosol deposition (AD) for the application of energy conversion systems.

For a sustainable energy supply sun, wind, and water are essential components. In addition to these energy sources, however, there are also some other renewable energies. For example, the vibration of buildings or the movement of people can be converted from mechanical to electrical energy by piezoelectric materials. This is called piezoelectric vibrational energy harvesting.

A piezoelectric vibrational energy harvester (PVEH) can consist of a substrate and a piezoelectrical material. Since piezoelectric ceramics exhibit very high piezoelectrical coefficients, they are excellent for the usage in PVEHs.

The most used piezoelectric ceramic on the market is lead zirconate titanate (PZT). Because of the damage to people and environment from production over usage to disposal of lead containing materials, lead-free alternatives are investigated. The most promising of those are barium calcium zirconate titanate (BCZT), potassium sodium niobate (KNN) and bismuth sodium titanate (BNT) based materials. In this project BCZT followed by KNN are in the focus of research.

Since ceramics need sintering i. e. a high temperature treatment to be fabricated, which exceeds the melting temperature of other material classes, it is hard to combine a ceramic piezoelectric with a non-ceramic substrate. This problem can be overcome with AD. With this technique various materials e. g. ceramics, glasses, metals, semi-conductors, or polymers can be sprayed onto different substrates at room temperature. Since no sintering is needed, metal or polymer substrates can be coated with a ceramic.

In this method an aerosol is generated by a carrier gas passing through loose powder in a vibrating chamber. The around one micrometer sized particles are transported driven by a pressure difference and accelerated through a nozzle into a vacuum chamber and onto a moving substrate. There the particles break apart into nanometer sized fragments and build new connections with the substrate and each other forming a dense film.

However, in the as-deposited state the functional properties of the AD films are much lower than in bulk samples. This might be due to their low grain size, since e. g. the permittivity and the piezoelectric coefficient are depending on that parameter. Therefore, an annealing step is needed to activate the high properties. For achieving this the sample can be annealed in a furnace, where all of the sample is heated up and grain growth should be triggered. To protect the non-ceramic substrate from the heat, only the AD film could be annealed by laser annealing.

Conclusions, main achievements and outlook

BCZT powders were produced via solid state synthesis and characterized regarding their crystal structure. Their particle size was varied by milling, so they could be used for AD. The temperature-dependent permittivity of a sprayed BCZT film was measured up to 500 °C under different atmospheres. The obtained curves were typical for AD films exhibiting e. g. a doubled permittivity value at room temperature after one heating cycle compared to the as-deposited film. This room temperature value is retained independent of the number of cycles applied after that. P-E hysteresis loops were measured from films annealed at 600 °C in air. The curves measured from 25 °C to 150 °C showed similar behavior like bulk samples above the curie temperature (Tc). The direct piezoelectric coefficient (d33), which is one of the most important parameters for energy harvesting, was measured after Corona poling with an Berlincourt meter, but sufficient d33 values could not be achieved till now. In both cases the reason might be the low grain size of AD films, which needs to be optimized.

To induce grain growth furnace and laser annealing were conducted. BCZT films sprayed on stainless steel were annealed in vacuum at temperatures from 500 °C to 900 °C. Since no improvement of the d_{33} could be observed, the annealing temperature was increased up to 1100 °C. For these high temperature experiments NiCr alloy was chosen as substrate, because stainless steel could not be used at these temperatures. The results still need to be analyzed. In parallel laser annealing tests were conducted on barium titanate (BT) AD films, because the efficiency of the BCZT powder still needs improvement. The influence of the laser parameters, especially of its current and scanning speed, were investigated by XRD and permittivity measurements. Regarding the crystallite size a slight trend for bigger sizes with higher current can be observed. The permittivity at room temperature also increased with increasing laser current linear from the value observed at an as-processed film to approximately half of the value of a furnace annealed film. The influence on the d_{33} will be investigated in the next measurements.

In cooperation with NITech the microtexture of an as-deposited and an at 500 °C in O_2 annealed AD film were investigated with Transmission electron microscopy (TEM). The size of the few existing crystals could be estimated to be ~5-100 nm. Most of the material consisted of an amorphous structure. This might be the reason for the low functional properties.

Since the storage of harvested energy would be an interesting feature of energy harvesters, the energy storage properties of BCZT bulk samples were investigated. It also makes sense to analyze AD films for the same purpose, because on these high electric fields can be applied, leading to high energy densities. The energy storage density and efficiency were analyzed in dependence of mechanical load, temperature and BCZT composition. An improvement of both parameters could be observed.

In project A, lead-free piezoelectric samples, which are planned to be produced in our lab, are integrated into a shoe to investigate their energy output by walking. Additionally, impedance spectroscopy measurements of the used materials will be conducted in our lab. From these the collaborators will derive an electrical model consisting of inductors, capacitors, and resistors. This will be used in the electrical circuit of the shoe and improve our impedance analysis.

Dielectric and ferroelectric experiments on BT and BCZT are done in cooperation with project D. Furthermore, the experience of conducting these will be exchanged.

In project H, bulk BCZT samples were analyzed e. g. in terms of crystal structure, pressure-dependent piezoelectricity, and temperature-dependent ferroelectricity. Since the same powder was used for these samples the results can be compared to our AD films and vice versa.

In cooperation with project I, ZrS_2 powder was deposited via AD onto silica glass and Si-wafer substrates. On these films a layer of BaS is planned to be deposited via electron beam evaporation to form the chalcogenide perovskite $BaZrS_3$. This will be investigated for the usage in optoelectronic devices.

Furthermore, the collaborative project was conducted with project A (Japan), C and E.

In cooperation with NITech the microtexture of an as-deposited and an at 500 °C in O_2 annealed AD film was investigated with Transmission electron microscopy (TEM). The size of the few existing crystals could be estimated to be ~5-100 nm. Most of the material consisted of an amorphous structure. This might be the reason for the low functional properties.

The collaboration will be increased in 2021 for preparation and conducting the research stay at NITech. When samples with a d_{33} usable in an energy harvesting device are obtained, these will be investigated in NITech in the lab of Prof. Kakimoto. An own equipment to characterize the energy harvesting behavior will be built in FAU. The processing technique spark plasma sintering will be used at NITech to investigate the influence of grain size on energy harvesting.

G - Formulation and Crystallization of Perovskite Bearing Glass-Ceramics for Light Management

FAU: Rita Cicconi and David Dobesh
NITech: Tomokatsu Hayakawa and Koichi Hayashi

Objectives and status

The objective of the project is to synthesize and characterize the formation of non-centrosymmetric crystals from within a glass matrix, forming a glass-ceramic. Glass synthesis through conventional melt and quench techniques allow for cost-effective and scalable parameters for industrial production. Compositional effects to the glass host will provide the pathway to ferro and piezoelectric crystals and investigate the influence of the residual surrounding glass matrix. The glass to crystal evolution will be studied through thermal treatments by varying temperature and time dependencies. Tailoring the composition of specialized components for the parent glass and active crystals will be of utmost importance. Glass structure connectivity from selective components will influence the type crystallinity and competing factors leading to their formation. The development of the crystal precipitation will be coupled with fundamental atomic bonding characters of the thermal and time variables to develop lead-free perovskite crystal structures.

Property analysis of the glass-ceramic for electro-optical and mechanical behavior will determine the evolution of the residual glass architecture and crystal size influences. Characterization of the glass to crystal structure was accomplished through investigations of the thermodynamic driving forces. Time and temperature variations on pristine glass samples provide an alternative synthesis route compared to conventional single and polycrystal production methods. The progression of nucleation and crystallization mechanisms from the glass matrix will allow for the advancement of crystal orientation and size dependencies. Precipitated crystals were characterized for their size influences on the refractive index, absorption, and emissions profiles due to alterations of chemistry and thermal parameters. The inclusion of glassy phase after thermal treatments may also provide coupling of a glass matrix for optimizing ferroelectric domains. Inclusions of rare earth element doping will also be investigated for the influences of polling on the upconversion emission profiles and lifetime decay profiles.

Current research has been undertaken through chemistry development to optimize glass-ceramics, which contain a ferroelectric, piezoelectric, and pyroelectric response. Components of the glass systems was selected to crystalize ferroelectric and pyroelectric phases from the base glass composition. Raman measurements of the parent glass compositions yielded changes in the short Ti-O apical oxygen bond and Q3 units with the chemical alterations. Complications of additional phases and a low degree of crystallinity influenced the difficultly for a phase identification through XRD detection limits. Literature reports of similar glass-ceramics have been studied to view their viability and reproducibility. However, selective reports of initial phases are being investigated and currently working towards a more comprehensive result. Our results demonstrate a systematic and controlled thermal process for thermal treatments to correlate time and temperature influences. The result of crystal clamping within the glass matrix and orientation of domain structures within the crystal sites will continue to be the research route. Controlling the glass to crystal structure for influences from components to the microstructure and ideal phase formation.

Familiarity and training were also accomplished with characterization equipment used for probing the glass and crystal structures. One such device is the ARABICA system, which training has been done for the set-up and alignment of optical components. The benefit of the system is to use inelastically scattered light to view the vibrational modes in the optical and acoustic branches and coupling with a DSC or hot stage for in situ measurements. Familiarity will help collaborations with other institutions and groups within the department.

Conclusions, main achievements and outlook

The synthesis of six base glass systems has been accomplished with particular components for thermal treatments. The initial base glass was selected due to the report of an initial phase of barium titanate. Adjustments to the components included the substitution of calcium for sodium to investigate the cation influence on the glass structure and crystal evolution. The replacement allowed the study of apparent surface crystallization from devitrification or the uncontrolled cooling rate from the liquidus temperature and thermal gradients. The surface crystal formation yielded surprisingly ordered patterning and spatial distribution of crystals. The methodology of the calcium replacement was for increasing the piezoelectric coefficient with cation or glass modifier replacement. Investigation of surface tension and stress between the crystal and glass interfaces was accomplished through optical birefringence and Raman spectroscopy mapping with different laser excitation sources for vibrational and bonding ranges. Calculations of the glass-forming ability from the substitution supplied the mixing of the alkali and alkali earth components to provide a stable glass network. Combining the two components promoted the desired melting and forming methods to have a composition that would contain electromechanical crystal phases in the form of barium titanate and barium calcium titanate.

Building upon the tailored glass composition, the inclusion of zirconia was added by adjusting the titania molar ratio. The addition of zirconia was to achieve a BCZT crystal phase as a precursor and act as a nucleating agent. Local bonding within the glass structure was analyzed to view the influence of the replacement of titania and the change in coordination number within the glass system. Zirconia has a character of a network modifier within the glass structure. Additionally, the incorporation allowed the chemical mapping of the zirconia content to view the glass-forming ability and surface crystallization. Adjusting the molar ratio of Zr/Ti also permitted the investigation of nucleating agents for thermal treatments. The upper limit of solubility of zirconia was established as 7 mol % with the direct substitution of titania. Surface crystallization of the upper limit displayed similar patterning as compared to the calcium containing parent glass. The patterning may be due to the thermal gradient when casting the molten glass on a brass plate with different cooling rates due to the volume of glass. The investigation is to study the degree of the preferred orientation and chemistry of the glass matrix surround the crystal to determine the movement or diffusion of cations and their effect on the crystal precipitation. One determined phase was fresnoite in the calcium substituted base glass system. The Pyroelectricity will be investigated to view the influence of the surface crystallization and comparison to the single crystal properties. Thermal treatments of the surface crystal orientations may provide insight into the crystal growth mechanisms from the surface to the bulk. The piezoelectric crystallite orientation and distribution may improve the connectivity through synthesis methods to optimize the piezoelectric response.

The parent glass compositions were analyzed using DSC to determine the glass transition, crystallization, and melting temperatures. Temperatures between the endo and exothermic reactions within the samples gave the thermal treatment window and investigation of the glass stability and provided the possible phase separation evaluations at the melting temperature. Varied heating rates were applied to extract the activation energies for the crystallization temperatures based on the Kissinger and Owaza methods. The Avarmi parameters also eluded to the type of crystallization in the form of homogeneous or heterogeneous formation. Optimization of the DSC parameters of glass particle size was also considered for adjusting the surface area of the prepared powders and pellets. The pellets were formed to compare the coupling of the sample surface to the DSC pan and thermal piles. The substituted components were also analyzed using DSC to view the shift in thermal energies. The coupling of the thermal data and heating rates lead to the development of thermal treatments for the parent glass compositions.

Calibration of thermal ovens was completed to provide constant thermal treatments and sample loading conditions and a selection of the base substrate using platinum foil rather than alumina plates, which may induce crystallization. Annealing and tube furnaces were also studied to view temperature gradients and thermal couple readings to produce accurate temperature treatments. Surface analysis of the thermally treated samples was done through optical and spectroscopic characterization. Influences on the number of crystals to the absorption and UV-cutoff will provide extrapolations to the bandgap energies. The electro-optical impacts will be considered by correlating the optical and dielectric measurements. The surrounding glass matrix will also be explored to determine the local pressure surrounding the crystals.

Future work is on the chemical diffusion and influence of the glass structure from time-temperature transformations. Viscosity measurements are currently being considered for extrapolating the viscosity behavior to correlate the diffusion of ions within the glass matrix. The piezo and ferroelectric properties will begin when geometric samples are suitable for dielectric behavior characterization. Controlling the nucleation and crystal size will be essential to compare the influence of the active electro-mechanical crystals.

Secondary and additional phases will also be investigated to view their contribution to electro-mechanical and electro-optical coupling. Additions to the parent of rare earth elements will be added to adjust the emission behavior and influence on the crystallinity. The crystal size and distribution will also be taken into account for optical transparency and adjustments for crystal site substitution.

Communication with NITech PIs was accomplished to introduce and determine research pathways through an online meeting and presentation. The research direction was discussed on current compositions and crystallization parameters. Prof. Hayakawa provided prospects of expanding the current direction of rare earth element incorporation of erbium to the possibility of co-doping with dysprosium for white light generation based on emission profiles. Additional niobate systems were also discussed based on the research and direction from advising a bachelor study this past year. Optical properties and local coordination of niobium within the aluminosilicate systems may provide a foundation for investigating the local coordination through XAFS and Raman characterization. We have also discussed collaborations for characterization methods available at NITech, such as optical measurements for Z-scan methods and NMR for local speciation, based on the availability of isotopes and magnetic field strengths for correlating the coordination numbers to structural relaxation of the glass to crystal evolutions. We have also discussed the incoming doctoral researcher at NITech for the collaboration of Project G. The NITech collaboration will be investigating the comparison of sol-gel synthesis routes. The viability and chemical compositions will help determine and compare structural influences on glass compositions through the melt quench and sol-gel methods. The synthesis will lead to the investigation of the chemical space and solubility of components. Additionally, the hydroxyl groups from the sol-gel process will be compared in the different synthesis routes.

External collaborations with Alfred University are also underway for investigating femtosecond laser modification of calcium aluminosilicate glasses. We are currently using the ARABICA system to look at the densification and modification of the glass structure. Laser irradiated regions are probed and compared to pristine regions to simultaneously collect the optical and acoustic modes through inelastic scattering with Raman and Brillouin Spectroscopy. The shift in the Brillouin spectra will be correlated for possible densification and artifacts that are a result of the laser interaction. The femtosecond laser irradiation may lead to temperature gradients in relaxation of the glass structure and alterations of the fictive temperature. The expansion of the collaboration is to increase the viability of current characterization equipment and facilitate collaborations within the scientific community.

H – Stress Modulated Electromechanical Coupling of Lead-Free Ferroelectrics

FAU: Kyle G. Webber, Ahmed Gadelmawla and Neamul Khansur
NITech: Koichi Hayashi and Yuta Yamamoto

Objectives and status

This project aims to experimentally investigate the influence of lattice defects and stress on the electromechanical properties and crystal structure of lead-free ferroelectrics for energy conversion systems through a combination of macroscopic measurements and local structure characterization. In particular, x-ray fluorescence holography at SPring-8 will be used to provide 3D atomic images around specific elements, giving information on the local lattice distortions and atomic fluctuations around dopants in disordered systems. Besides, x-ray diffraction with resonant scattering, x-ray absorption fine structure, and inelastic X-ray scattering will also be employed to understand local structure and phase transitions of lead-free ferroelectric materials.

Conclusions, main achievements and outlook

Lead-free ferroelectric BCZT was synthesized and characterized with lab X-ray diffraction and Raman spectroscopy (see Figure 1) in collaboration with IRTG project G (Dr. Maria Rita Cicconi and David Dobesh). Furthermore, the influence of stress on the phase boundaries of BCZTx was characterized with small-signal relative permittivity and direct piezoelectric coefficient from −150 to 200 °C under uniaxial compressive stress up to 75 MPa (see Figure 2).

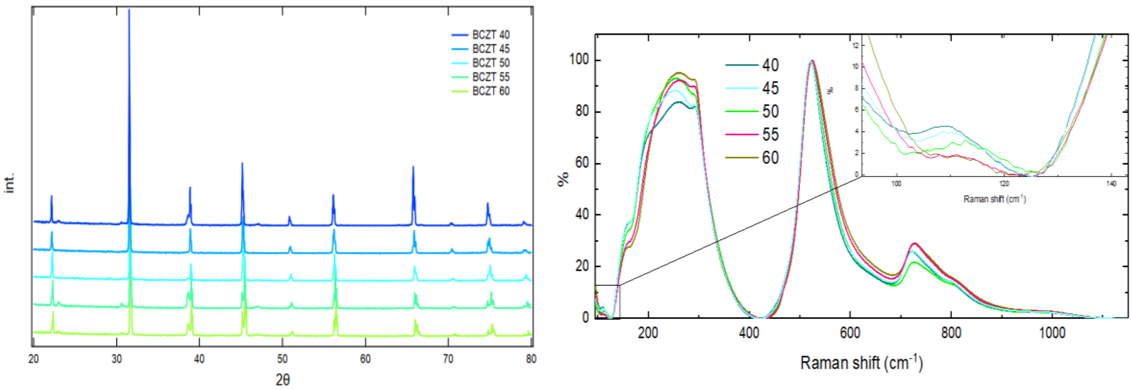


Figure 1. Lab X-ray powder diffraction (left) and Raman spectroscopy (right) of BCZTx (i.e. x = 40, 45, 50, 55, 60).

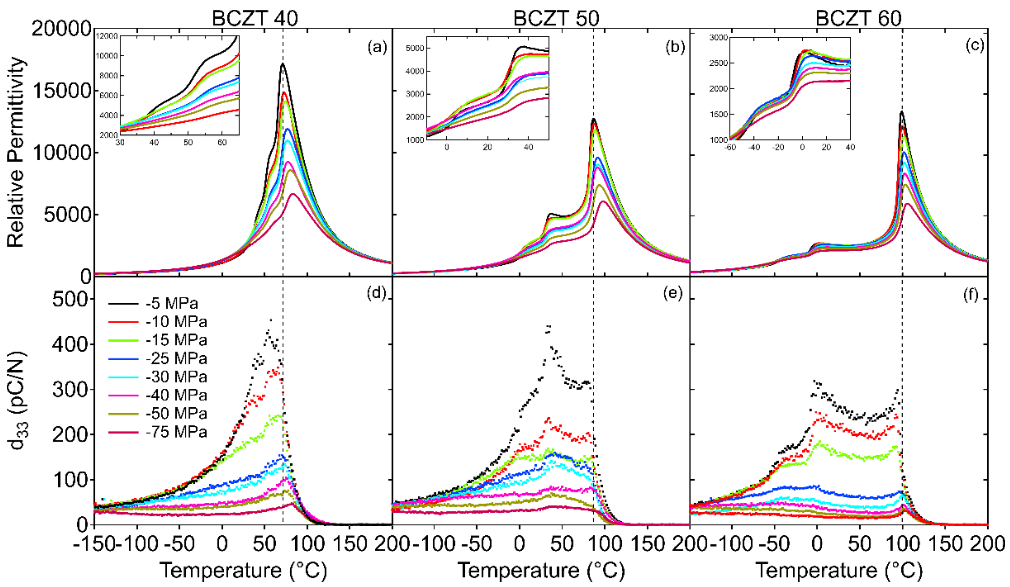


Figure 2. The temperature-dependent ε_r (10 kHz) (a, b, and c) and d_{33} (110 Hz) (d, e, and f) as a function of uniaxial compressive stress within the range from −5 MPa to −75 MPa of BCZT40, 50, and 60, respectively.

In order to correlate the macroscopic properties to the local structure of BCZT, the samples were sent to NITech to be prepared and will be measured at SPring8 with x-ray fluorescence holography to provide 3D atomic images around the elements. However, prof. Hayashi group with x-ray fluorescence holography and inelastic X-ray scattering will also measure some of the BCZT single crystals from prof. Qingfeng group, Tsinghua University, China. The rest of the BCZT single crystal will be measured at ESRF with temperature-stress dependent single-crystal X-ray diffraction to determine the phase transitions as a function of stress and temperature.

I - Growth of Single Crystal Transition Metal Perovskite Chalcogenides

FAU: Peter Wellmann and Tim Freund
NITech: Koichi Hayashi and Reina Miyagawa

Objectives and status

The goal of the nine-year project is to synthesize and manufacture optoelectronic devices based on single crystals or epitaxial layers of Chalcogenide Perovskites.

To eventually achieve this, the goal of the first three-year doctoral project is to establish routes for the fabrication of polycrystalline thin films of $BaZrS3$ (BZS) and related materials and to examine their optoelectronic properties as well as to acquire thermodynamic and thermokinetic data for those materials. The main goal of the first year of the project was to demonstrate the fabrication of BZS thin films from Stacked Elemental Layers (SEL). This technique is common practice for the production of solar cells made from Cu(In,Ga)Se2 (CIGS), Cu2InSnS4 (CZTS) and similar, chalcogenide materials.

Therefore, using an Edwards E306A Electron Beam Coating System, subsequent precursor layers of Zr and BaS were successfully evaporated onto glass substrates. The layer thickness was in the range of several hundred nanometres and was adjusted, so that they roughly represented the 1:1 Ba:Zr ratio needed for the formation of BZS. Those samples were annealed in a tube furnace at 500°C for up to 20 hours. Both possible stacking orders were tested throughout all annealing experiments. At this temperature, no signs of a reaction between the layers was observed and thus, experiments at higher temperatures were conducted. To do this, silica glass was used as a substrate, as glass can only be used for temperatures up to 500°C. A multitude of annealing experiments were done with temperatures up to 900°C. However, still no sign of a reaction between the layers occurred. As this was the maximum temperature that could be reached using the tube furnace in use, instead an induction oven originally intended for the growth of SiC using the physical vapor transport method was used to achieve even higher temperatures. Additionally, another substrate switch was necessary as the maximum usage temperature of silica glass is around 1000°C. It was decided to utilize polycrystalline SiC pieces readily available in our research group. Those samples were annealed at temperatures of 1000°C and 1200°C in a graphite crucible with the addition of elemental sulphur. However, BZS still was not the main constituent of the resulting sample.

In order to do more experiments at temperatures up to 1600°C, it was decided to setup such an induction oven dedicated to these experiments, as the one previously mentioned is primarily used in other fashion. Fortunately, such a device was available within the research group and was installed at the facility. Currently, the setup process is being executed as well as the installation of a pyrometer capable of measuring at temperatures below 900°C, which was the lower limit of the previously employed device. This lower temperature regime is important, as the boiling point of elemental sulphur is roughly 444°C.

Additionally, two other methods for the deposition of precursor films are currently under exploration:

1. First, in cooperation with Project F, Aerosol Deposition (AD) has been recently used for the deposition of ZrS2 powder onto silica glass and Si-wafer substrates. However, due to technical difficulties with the Electron beam evaporation setup, the subsequently planned deposition of BaS and annealing of the resulting sample has not been done yet.

2. Second, an electrodeposition (ED) setup has been installed at the facility, and is currently in use for the deposition of ZrSe2 layers. ED is another common method utilized in the fields of CIGS and CZTS.

Conclusions, main achievements and outlook

In order to synthesize BZS thin films using the SEL method, the deposition of precursor layers has been successfully established using electron beam evaporation. The research on alternative deposition methods, namely ED and AD, has been initiated and will be under investigation in the upcoming months. As the previously used temperatures in the annealing of the deposited layers is insufficient for the successful synthesis of BZS, equipment solely dedicated for this processing and experiments at temperatures of up to 1600°C will be in use in the near future to eventually successfully fabricate BZS thin films.

Other options that will be under investigation are the potential direct deposition of the ternary chalcogenide compound using ED, as well as the synthesis of other compositions of the chalcogenide perovskite material class.

Furthermore, in cooperation with the Japanese investigators, the potential use of the manufactured layers in water splitting, as well as the epitaxial growth using laser pre-structured substrates and in-depth investigation of the defects in the material should be explored within the framework of the first doctoral research project.

J - Solution Processed Ferroelectrics in Photovoltaic Devices

FAU: Wolfgang Heiss, Viktor Rehm and Mykhailo Sytnyk
NITech: Shinji Kawasaki and Yosuke Ishii

Objectives, main achievements and status

The development of metal halide perovskites has revolutionized the field of solution processed solar cells. It is obvious that the performance of solar cells and other electronic devices crucially depends on defects, present in bulk, and increasingly at surfaces and grain boundaries. Hence, single - crystal devices usually outperform polycrystalline and amorphous ones, which is also observed for the metal halide perovskites. Thus, our group has developed the deposition of metal halide perovskite single crystal layers by epitaxial growth from solution. In particular in this work, which was performed in collaboration with the IRTG projects of C. Brabec and P. Wellmann, epitaxial microcrystals and continuous films were obtained by ink-jet printing of various metal-halide perovskites on various substrates. We have identified several important parameters to obtain epitaxial growth from the solution, such as lattice mismatch, substrate temperature, surface activation, and environmental humidity. The epitaxial structures showed not only coherent interfaces to the substrates, but provided also outstanding optical properties. A benefit of the epitaxial growth was also that the lattice of the perovskite is stabilized by the substrates, so that the cubic room temperature phase of MAPbBr3, for instance, could be observed over a wider temperature range.

The associated researcher of this project is making use of the defect-tolerance of metal-halide-perovskites and based on that he is developing highly luminescent perovskite nanomaterials, by embedding them into an epitaxial matrix. The matrix improves the luminescence efficiency drastically as well as the environmental stability. An important feature is also that the matrix is optically highly transparent, so that from these materials eventually solar-concentrators or similar devices could be developed in the future.

The group of the Japanese Co-PI has performed several important steps towards the fabrication of electron transport layer materials, representing an essential part of a solar cell. They have installed an ultra-centrifuge system in their lab for the separation of metallic and semiconducting single wall carbon nanotubes (SWCTs) by the density gradient centrifuge separation method and the success of the separation was confirmed by absorption spectroscopy. Furthermore, they have attempted to scale up the synthesis of fluorinated fullerene materials, which are interesting materials for applications in electron transport layers of the solar cells. Furthermore, some activities were performed which will be of relevance for the next funding period of the IRTG.

The performed work is related to CO2 reduction on one hand and to solar H2 generation on the other hand. This work is performed with an organic pigment, epindollidione, (EPI) which was initially delivered by our group. For CO2 reduction the co-PIs group developed a new method to prepare metal nano-particles (Ni and Cu , <10 nm) on SWCNTs by using metal-complex molecules encapsulated in SWCNTs. They converted Ni to Ni(OH)2 and investigated its battery electrode properties. They also investigated solar CO2 reduction catalytic properties of Cu/SWCNT/EPI compounds. While initial experiments with EPI evidenced some instability of this material, the co-PIs group found that, if they used metal co-catalyst, no degradation of EPI was observed by SEM for solar H2 generation. They have tested some kinds of metals which can work as co-catalyst and they have prepared a flexible transparent catalyst electrode using graphene.

The doctoral researcher of this project is working on solution processed ferroelectric perovskites for the use in solar cells. The aim is to use the intrinsic polarization of such materials in order to enhance the charge separation and thereby the overall power conversion efficiency of such devices. A first candidate with the name Butylammonium-Methylammonium Lead Bromide (BA2MA2Pb3Br10) was chosen and synthesized in form of polycrystals and single crystals as well as in form of thin films. The materials show bright photoluminescence and high stability regarding oxidation and humidity. However, due to their biaxial nature the measurement of Polarization-Electric field (P-E) hysteresis of polycrystalline samples still remains elusive. This measurement is necessary to distinctly prove the ferroelectric nature of the material and ideally should be done on single crystals. Therefore, in order to get high quality and large crystals we are still working on a new setup for crystal growth. Furthermore, electrical characterization of the material revealed nonlinearities, that are alluding to the ferroelectric properties of the compound. In the end, nanocrystals of the same compound were synthesized using three different techniques. This includes direct synthesis via hot injection and a two-step approach, where at first PbBr2 nanocrystals are synthesized and subsequently transformed via intercalation to the desired composition. Lastly, the ligand-assisted reprecipitation (LARP) technique, that is often used for conventional perovskite halides was also developed for the ferroelectric perovskite. All of the described methods resulted in nanocrystals with tunable size and bright photoluminescence. Unfortunately, these nanocrystals show only moderate colloidal stability when compared to traditional inorganic nanocrystals and can degrade or aggregate if not handled carefully.

Conclusions and outlook

The research idea was to choose one ferroelectric perovskite compound, that is already described in literature and replicate the results. With the newly gained knowledge of syntheses and properties of such compounds a new ferroelectric molecular perovskite material was to be developed. However, during the research it became clear that all of the published ferroelectric perovskites have a wide band-gap, therefore limiting their use as an absorber in photovoltaics. Fortunately, the materials that were synthesized may still be used in tandem solar cells or as photodetectors. Additionally, during the year it was shown that the material MAPbI3, which is the most studied perovskite halide, used as the absorbing layer in solar cells, is indeed ferroelectric. Such good news inspired us to develop single crystal solar cells out of this material in the coming year starting from January. We are very interested and eager to see and investigate how the ferroelectric properties of the MAPbI3 can influence performance and efficiency of such devices.

The work on epitaxial growth of metal halide perovskite by inkjet printing has been performed in collaboration with the projects of C. Brabec and P. Wellmann. Furthermore, we have been collaborating with the project of K. Webber, on a paper on plasmonic electrochromic effects in nanocrystal based devices operating in the infrared spectral range.

So far the collaboration with NITECH is restricted to exchanging emails and materials. This allows to develop the various materials for the solar cells in an independent way and the will be combined in a later stage of the project.

K - Multi-Scale Modeling of Electromechanical Coupling in Perovskite-Based Ferroelectric Materials and Composites

FAU: Michael Zaiser, Frank Wendler, Sai Prasanna Veluri and Asutosh Padhy
NITech: Shuji Ogata and Takahiro Tsuzuki

Objectives and status

To enable a simulation of ferroelectric domain evolution under external electrical and mechanical loading, a phase-field model based on an enthalpy density description was developed. In the first year of the project, the focus for the FAU project team was set on the continuum model and development of a maintainable and scalable code. A coordinate invariant model based on the approach of [D. Schrade, Int. J. Solid. Struct. 51/11 (2014) 2144] was formulated and implemented in Numerical Python using a semi-implicit pseudo-spectral FFT scheme. The coupled electro-elastostatic equations are solved using an FFT based homogenization scheme.

As a first model system the ferroelectric perovskite BaTiO3 was chosen due to availability of reliable potential parameters for molecular dynamics. For the intended coupling of simulations on the atomistic scale (NITech group) with the continuum model from the FAU team the exchange of several physical parameters are important, that have to be extracted from the molecular simulations. The NITech team worked on methods to calculate the barrier free energy of the ferroelectric domain boundary during motion in addition to the interface energy for realistic settings. Effects on the free energy barrier by the polarization direction, defects, temperature, etc. will be considered in future. The mobility of domain boundary as another key parameter can be evaluated from the barrier free energy.

The NITech team extended the original molecular dynamics simulation code using the shell model inter-atomic potential [Vielma and Schneider: J. Appl. Phys. 114, 174108 (2013)] for BaTiO3. The shell model regards an atom as to be composed of the shell (mimicking valence electrons) and core (the remaining); the shell position is dynamically determined from the minimum total energy. A novel meso-scale control method for the domain boundary motion, coined as coarse-grained particle (CGP) method, was formulated for the MD simulations. The NITech team has succeeded to implement the CGP method to the MD code and has started its preliminary usage.

Conclusions, main achievements and outlook

In the phase-field code, relaxor behavior was introduced as single or combined effect of random bond and random field contributions. Random bonds are simulated by varying the coefficient of the harmonic part of the Landau potential. Random fields are included in the solution of the equilibrium equations. It was shown that the presence of random bonds strongly enhances the effect of an imposed random field. Fig. 1 a shows the evolution of disorder in the domain pattern when the random field is increased from 0.5 to 1.5 EC (from left to right).

Concerning MD methods, the ferroelectric domain boundary usually moves too slowly under conventional fields. Therefore, extremely strong electric fields were imposed in former simulation studies despite unphysical atomic dynamics. The NITech group worked on a novel idea to control domain boundary motion under realistic conditions by introducing coarse-grained particles (CGPs) to macroscopically control the atomic polarization. Each CGP controls the atoms in a specified region. Seamless control of the atoms is realized by overlapping the specified regions; overcontrol in the overlap region exactly cancels out. To realize the idea, the NITech team first produced original MD code for BaTiO3, which is parallelized for fast computation in a supercomputer. Second, they implemented the CGP method to the MD code. Fig. 1 b demonstrates the domain motion observed in the MD simulation with the CGP method. Red or blue arrow indicated the polarization of each unit cell; color represents the y-component. The red domain shifted toward x-direction by about three unit cells.

The NITech team is presently adapting the parameter values in the CGP method. In year 2021, MD simulations with the CGP method to obtain the barrier free nenergy during domain wall motion of BaTiO3 in various realistic settings is planned. The results will be used in the phase-field modeling in the FAU team.

a)

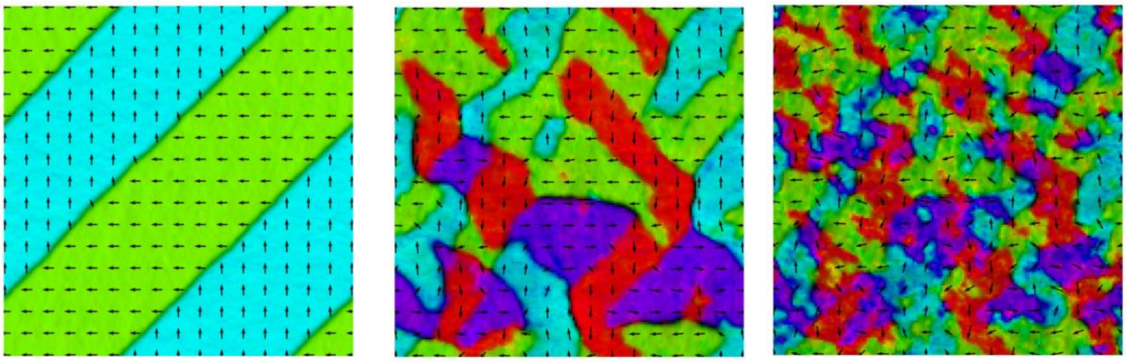


Figure c Stable domain patterns (phase-field) under increasing random field from left to right (mechanically clamped, short circuited).

b)

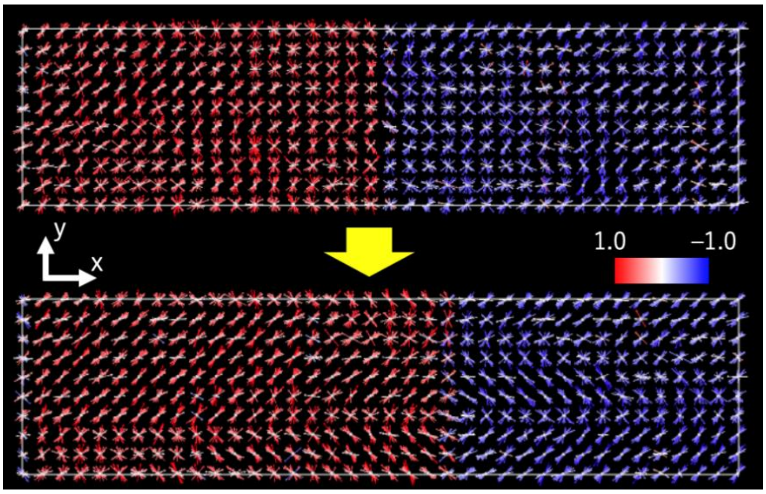


Figure d Ferroelectric domain boundary motion in x-direction observed in the MD simulation of BaTiO3 with the CGP method. The colored arrow indicates polarization and magnitude (wrt to y-direction) of each unit cell.

L - Modeling of Defect and Surface Chemistry of Perovskites

FAU: Bernd Meyer, Samuele Spreafico and Christian Ritterhoff
NITech: Masaaki Haneda

Objectives and status

In this project, we use atomistic quantum-mechanical methods based on density functional theory (DFT) to study electro-optical, electro-mechanical and surface-chemical properties of perovskite materials. Specifically, projects on four different topics were started in 2020: Samuele Spreafico performed first DFT calculations on the atomic and electronic structure of promising halide perovskites for solar cell application, with the long-term goal of his PhD work to get a better understanding of their defect tolerance (collaboration with Project E, Brabec, and Project J, Heiss). The topic of the Master Thesis of Bernd Schmidt is to study the strain dependence of the re-orientation energy and activation barrier of defect dipoles in $SrTiO_3$ and related ferroelectric perovskites (collaboration with Project H, Webber). The group of Prof. Haneda uses the adsorption of probe molecules to identify special surface sites on catalyst surfaces by measuring characteristic shifts in their vibrational frequencies with IR spectroscopy. To support the interpretation of these experiments, Simone Reindl calculated the vibrational signature of methanol molecules adsorbed on a series of ideal, defective and doped oxide surfaces for her Bachelor Thesis. Finally, as part of his PhD work Christian Ritterhoff implemented a new method for localizing wave functions in DFT calculations, which will allow us to reduce the computational cost of hybrid functional calculations in future studies on the electronic properties of perovskite materials.

Conclusions, main achievements and outlook

In a first series of calculations, Samuele Spreafico determined the lattice parameter, electronic structure and band gap of $CsMX_3$ halide perovskites for a systematic series of M-site substituents and the halides Cl, Br and I, assuming a simple cubic perovskite structure. The investigated $CsMX_3$ perovskites can be divided into three groups according to their band gaps (see Fig. 1): semiconductors with an appropriate band gap for solar cell application, insulators with a too large and metals with a vanishing band gap. The bromides of this series were synthesized in the group of Prof. Heiss. The aim was to stabilize the cubic structure of the perovskites by embedding them as nanoparticles in a cubic CsBr matrix. The measured photoluminescence, which is an indicator for defect tolerance, nicely correlates with the results of Fig. 1 (though it is not guaranteed that indeed perovskites in the cubic structure had formed in the experiments): the materials predicted by theory to be metallic did not show any photoluminescence at all, whereas the strongest signal was observed for the semiconducting ones. The results were then refined by optimizing the experimentally known room temperature crystal structure of the perovskites and by calculating the band gap with a more reliable (though computationally much more expensive) hybrid functional. As the next steps, atomic defects will be introduced into the crystal lattice of the most promising perovskite compounds and the electronic structure of the interface to the CsBr matrix will be investigated.

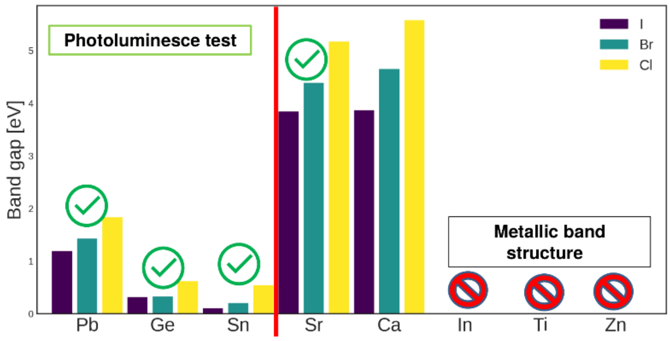


Figure 1 Calculated PBE band gaps for a series of cubic $CsMX_3$ perovskite compounds.

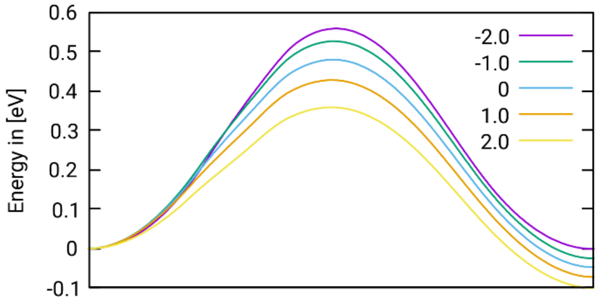


Figure 2 Energy profile for the migration of an O atom from an equatorial (left) to a longitudinal (right) position depending on the applied uniaxial strain (see

In the study of the strain-dependent properties of defect dipoles in $SrTiO_3$, first only O vacancies were considered. Bernd Schmidt calculated the energy difference between the equatorial and longitudinal position of the O vacancies and the activation barrier for the diffusion of an O atom between the two sites as function of an applied uniaxial strain (see Fig. 2). The results show a rather small strain dependence of the diffusion barrier and of the energy difference between the two vacancy sites. Since the absolute height of the barriers is also small, the distribution of the vacancies under applied strain will remain close to thermodynamic equilibrium. In the next step, a Ti ion next to the vacancy was replaced by Fe to create a stronger defect dipole complex. The calculations on the re-orientation energy and barrier are still in progress. The study will be extended to ferroelectric perovskites, such as $BaTiO_3$ and BCZT, in which the lattice is already distorted at room temperature without applying an external strain.

The main questions asked by Prof. Haneda are, if it is possible to distinguish between methanol molecules adsorbed on different crystallographic surfaces or next to surface vacancies and Zr dopant atoms by measuring their vibrational frequencies. To this end, Simone Reindl performed calculations of the vibrational frequencies of methanol adsorbed on three different surfaces before and after a vacancy and a Zr dopant atom were introduced. She showed that the surface orientation has only a minor impact, whereas Zr dopants lead to a significant shift in the C-O stretch frequency of 40-60 cm^{-1}. Unfortunately, severe convergence problems were encountered in the calculations with O vacancies, so that here no final statement could be made.

By localizing electronic states in DFT calculations, the overlap between most orbital pairs becomes almost zero, which allows to neglect many terms in the overall calculation. The benefit is particularly huge when hybrid functionals are considered. Here, the scaling of the most time consuming part can be reduced from cubic to linear with respect to the number of electrons in the calculation. Christian Ritterhoff has implemented successfully the method of the selected columns of the density matrix (SCDM) for the specific case of Vanderbilt ultrasoft pseudopotentials into the *ab initio* molecular dynamics code CPMD. This implementation is currently used to speed-up the evaluation of the Hartree-Fock exchange, which is the time consuming part in hybrid functional calculations. In the future, this will be combined with the adaptively compressed exchange (ACE) operator method, which is a second step to reduce the computation burden of hybrid functional calculations.

2.1. Participation in conferences

David Dobesh

From / to	Name of the conference	Location	Title of presentation or poster, or participation only
08.-10.09.20	EXAFS 2020 -SSRL Summer School on Synchrotron X-Ray Absorption Spectroscopy	online	Participation

David Köllner

From / to	Name of the conference	Location	Title of presentation or poster, or participation only
07.10.20	CellMat 2020	online	Presentation “Cellular structures with modified strut properties by replicating a 3D printed Polymer”

Christian Kupfer

From / to	Name of the conference	Location	Title of presentation/poster, or participation only
07.-09.12.20	NGSE5	online	Participation

Viktor Rehm

From / to	Name of the conference	Location	Title of presentation/poster, or participation only
07.-09.12.20	NGSE5	online	Participation

Samuele Spreafico

From / to	Name of the conference	Location	Title of presentation/poster, or participation only
07.-09.12.20	NGSE5	online	Participation

Jonas Biggemann

From / to	Name of the conference	Location	Title of presentation or poster, or participation only
26.-31.01.20	Advanced Ceramics and Composites International Conference (ICACC)	Daytona Beach, US	Presentation ”Automated 3D-Assembly of Modular Ceramic Composites Structures”

Neamul Khansur

From / to	Name of the conference	Location	Title of presentation/poster, or participation only
19.-23.07.20	IEEE IFCS-ISAF 2020	online	Participation
07.-09.12.20	NGSE5	online	Participation

Takeshi Okada

From / to	Name of the conference	Location	Title of presentation/poster, or participation only
14.-15.05.20	Joint Technical Meeting on "Motor Drive", "Rotating Machinery" and "Vehicle Technology"	Online	Participation
25.-27.11.20	23rd International Conference on Electrical Machines and Systems (ICEMS2020)	Online	Presentation “Design and Experimental Studies on HEFSM Employing Two Types of Permanent Magnets per Pole as Traction Motor for Automobile Applications”
24.11.-11.12.20	JMAG Users Conference 2020	Online	Poster presentation “Magnetization analysis for hybrid excitation flux switching motor employing variably magnetizable permanent magnets”

2.2. Publications

Published

[1] R. Hasegawa, **M. Mehnert, J. Mergheim, P. Steinmann, K. Kakimoto**: *Behavior of vibration energy harvesters composed of polymer fibers and piezoelectric ceramic particle*, Sensors and Actuators A: Physical, 303, 111699 (2020) [GRK B/C]
DOI: 10.1016/j.sna.2019.111699

[2] M. Chen, **J. Wang, D. Anzai, G. Fischer, J. Kirchner**: *Common-mode noise reduction in noncontact biopotential acquisition circuit based on imbalance cancellation of electrode-body impedance*, Sensors, vol. 20, 7140 (Dec. 2020) [GRK A]
Doi: 10.3390/s20247140

[3] **Cicconi MR**., **Khansur NH.**, **Eckstein U.**, Werr F., **Webber K.**, de Ligny D.: *Determining the local pressure during aerosol deposition using glass memory,* Journal of the American Ceramic Society103, p. 2443-2452 (2020) [GRK F/G]
DOI: 10.1111/jace.16947

[4] Mashkov O., Körfer J., Eigen A., Yousefi Amin AA., Killilea NA., Barabash A., **Sytnyk M., Khansur NH.**, Halik M., **Webber K., Heiß W**.: *Effect of Ligand Treatment on the Tuning of Infrared Plasmonic Indium Tin Oxide Nanocrystal Electrochromic Devices*, Advanced Engineering Materials (2020) [GRK F/J]
DOI: 10.1002/adem.202000112

[5] H. Nishiyama, **A. Martin**, K. Hatano, S. Kishimoto, N. Sasaki, **N.H. Khansur**, **K.G. Webber, K. Kakimoto**: Electric-field-induced strain of (Li,Na,K)NbO_3-based multilayered piezoceramics under electromechanical loading, J. Appl. Phys. 128(24) (2020) 244101. [GRK H]
DOI: 10.1063/5.0029615

[6] Lorenz MM., **Martin A., Webber K**., Travitzky N.: *Electromechanical Properties of Robocasted Barium Titanate Ceramics,* Advanced Engineering Materials (2020) [GRK H]
DOI: 10.1002/adem.202000325

[7] **Mykhailo Sytnyk**, Amir-Abbas Yousefi-Amin**, Tim Freund**, Annemarie Prihoda, Klaus Götz, Tobias Unruh, Christina Harreiss, Johannes Will, Erdmann Spiecker, Jevgen Levchuk, **Andres Osvet, Christoph J. Brabec**, Ulrike Künecke, **Peter Wellmann,** Valentin V. Volobuev, Jędrzej Korczak, Andrzej Szczerbakow, Tomasz Story, Clemens Simbrunner, Gunther Springholz, Daniel Wechsler, Ole Lytken, Sebastian Lotter, Felix Kampmann, Janina Maultzsch, Kamalpreet Singh, Oleksandr Voznyy, **Wolfgang Heiss:** *Epitaxial Metal Halide Perovskites by Inkjet-Printing on Various Substrates,* Advanced Functional Materials [GRK E/I/J]
DOI: 10.1002/adfm.202004612

[8] **Martin A**., **Khansur NH**., **Eckstein U., Rieß K., Kakimoto KI., Webber K**.: *High temperature piezoelectric response of polycrystalline Li-doped (K,Na)NbO3 ceramics under compressive stress,* Journal of Applied Physics 127 (2020), Article No.: 114101 [GRK F/ NITech]
DOI: 10.1063/1.5134554

[9] **Biggemann, J.;** Müller, P.; **Köllner, D.;** Simon, S.; Hoffmann, P.; Heik, P.; Lee, J.H.; **Fey, T.**: *Hierarchical Surface Texturing of Hydroxyapatite Ceramics: Influence on the Adhesive Bonding Strength of Polymeric Polycaprolactone,* Journal of Functional Biomaterials [GRK D]
DOI: 10.3390/jfb11040073

[10] Ening Gu, Xiaofeng Tang, Stefan Langner, Patrick Duchstein, Yicheng Zhao, Levgen Levchuk, Violetta Kalancha, Tobias Stubhan, Jens Hauch, Hans Joachim Egelhaaf, Dirk Zahn, **Andres Osvet, Christoph J. Brabec:** *Robot-Based High-Throughput Screening of Antisolvents for Lead Halide Perovskites*, Joule, Volume 4, Issue 8 (2020), p. 1806-1822 [GRK E]
DOI: 10.1016/j.joule.2020.06.013

[11] Myszka B., Schodder P., Leupold S., Barr M., Hurle K., Schüßler M., Demmert B., **Biggemann J., Fey T.**, Boccaccini AR., Wolf S.: *Shape Matters: Crystal Morphology and Surface Topography Alter Bioactivity of Bioceramics in Simulated Body Fluid,* Advanced Engineering Materials (2020) [GRK D]
DOI: 10.1002/adem.202000044

[12] **Khansur NH., Martin A., Rieß K**., Nishiyama H., Hatano K., Wang K., Li JF**., Kakimoto KI., Webber K.**: *Stress-modulated optimization of polymorphic phase transition in Li-doped (K,Na)NbO3*, Physics Letters 117 (2020), Article No.: 032901 [GRK H]
DOI: 10.1063/5.0016072

[13] **Khansur NH., Biggemann J.,** Stumpf M., **Rieß K., Fey T., Webber K**.: *Temperature- and Stress-Dependent Electromechanical Response of Porous Pb(Zr,Ti)O3,* Advanced Engineering Materials (2020) [GRK D/H]
DOI: 10.1002/adem.202000389

Submitted

[1] H Nishiyama, **A Martin**, K Hatano, S Kishimoto, N Sasaki, **KG Webber**, and **K Kakimoto**, *Alkali volatilization of (Li,Na,K)NbO3-based piezoceramics and large-field electrical and mechanical properties*, Journal of the Ceramic Society of Japan (2020) (accepted)

[2] A These, **NH Khansur**, O Almora, L Luer, GJ Matt, **U Eckstein**, A Barabash, **A Osvet, KG Webber**, and **CJ Brabec**, *Characterization of Aerosol Deposited Cesium Lead Tribromide Perovskite Films on Interdigited ITO Electrodes*, Advanced Electronic Materials (2020) (accepted)

[3] **Haque MI**, Yoshibayashi K, **Wang J, Fischer G, Kirchner J.** *Directive Antenna Design at 2.4 GHz on Foot Surface for Wanderer Location Identification,* International Symposium on Antennas and Propagation (ISAP2020). (accepted)

3. Qualification Concept

3.1. Qualification Program

The qualification program was developed to cultivate an inter-project scientific exchange and understanding and provide our members with a unique interdisciplinary learning opportunity. The program in 2020 comprises (i) the FAU-NITech School on Energy Systems, (ii) the FAU-NITech lecture series, (iii) the Collaborative Project on Integrated Coupled Energy Harvesting Systems, and (iv) an international guest program (invited colloquia), accompanied by integrated soft skills training.
The first year concentrates on introductory lectures on lead-free ferroelectrics, materials and devices for opto-electrics, and modeling techniques. Through feedback from doctoral researchers and PIs, this program will be continuously improved and refined.

Right at the beginning of our International Research Training Groups program, we were confronted with a worldwide pandemic that restrained our international team from meeting in person and traveling. From now on, we had to get accustomed to digital conferences, Zoom meetings, online seminars and working at home. At the university working was, and still is, allowed only under strict protective measures. This all, sadly, with no real end in sight.

However, by reorganizing the program to hosting mostly online events, in the end we ensured that everything was available online and on-demand, and created an extensive knowledge base online.

Kick-off Meeting (February 24th – 26th)
The first phase of the interdisciplinary collaboration and cultural exchange of our IRTG was opened by the Kick-off Meeting, where all members from FAU and NITech alike got together at the “Welcome Residenzschloss Hotel” in beautiful Bamberg. The participants were given an overview of industrial research activities in Germany on perovskite materials for piezoelectric and x-ray detection systems by two of our industrial advisors, Dr. Gunnar Picht from Robert Bosch GmbH and Dr. Oliver Schmidt from Siemens Healthineers. Following this, PIs from FAU and NITech introduced their proposed projects and held Ring Lectures on a variety of topics from ceramic processing and ferroelectricity to photoelectrochemical water splitting and single crystal growth. Moreover, all doctoral researchers joint the workshop on “Good Scientific Practice” held by Dr. Schmitt-Engel from the FAU Graduate Centre.
During joint dinners with traditional food, PIs, doctoral researchers, and associated researchers got together for scientific and cultural, and on the last day we enjoyed a beer tasting at a local Brewery and a guided sightseeing tour by two “locals” of Bamberg.



After the Kick-off meeting in the first year, the second and third year the participants of both institutes will get together at “Yearly Schools”- alternately in Germany and Japan. Doctoral Researchers are expected to join all three annual meetings.

Invited Lectures

In order to stay connected within the ferroelectrics community during the times of Covid 19, Prof. Kyle Webber, Tutorials and Education Chair of the Ferroelectrics Standing Committee of the IEEE UFFC, has organized a bi-monthly webinar series on various topics related to the processing, characterization, structure, or modeling of ferroelectrics – a total of 13 speakers in 2020 only! To cover also the electro-optical side of the IRTG, three more talks were organized.

Doctoral researchers should listen to at least 12 talks over the three years.

	Date	Speaker	Affiliation	Title
1	May 19	**Andrew Bell**	University of Leeds, UK	*How are the Electromechanical Properties of Ferroelectrics Interrelated?*
2	Jun 2	**Susan Trolier-McKinstry**	The Pennsylvania State University, USA	*History of ferroelectricity*
3	Jun 16	**Roger Whatmore**	Imperial College London, UK	*Pyroelectric Materials and IR sensing*
4	Jun 30	**Brendan Hanrahan**	U.S. Army Research Laboratory, UK	*Pyroelectric Materials for Energy Harvesting*
5	Jul 14	**Marco Deluca**	Materials Center Leoben Forschung GmbH, Austria	*What can I learn about ferroelectrics with Raman spectroscopy?*
6	Jul 28	**Paolo Colombo**	University of Padova, Italy	*3D printing of ceramics*
7	Aug 25	**Shujun Zhang**	University of Wollongong, Australia)	*Why relaxor-PT single crystals possess giant piezoelectricity?*
8	Sep 8	**Wook Jo**	Ulsan National Institute of Science and Technology, South Korea	*Lead-free piezoceramics and what more?*
9	Sep 22	**Neus Domingo**	Catalan Institute of Nanoscience and Nanotechnology, Spain)	*The adsorbates on Ferroelectric Surfaces: those long-ignored neighbors*
10	Sep 29	**Efrat Lifshitz**	Israel Institute of Technology, Israel	*Magneto-optical properties of Perovskite nanocrystals*
11	Oct 6	**Jacob Jones**	North Carolina State University, USA	*Quantifying domain wall contributions to properties using X-rays*
12	Oct 13	**Juan Morante**	Institut de Recerca en Energia de Catalunya, Spain	*What would it take for renewably based electro synthesis products to substitute those obtained from petrochemical processes*
13	Oct 20	**Manuel Hinterstein**	Karlsruhe Institute of Technology, Germany	*Structure-property relations in ferroelectrics*
14	Nov 17	**Jürgen Rödel**	Technische Universität Darmstadt, Germany	*Ferroelastic toughening in ferroelectrics*
15	Dec 1	**Alexander Colsmann**	Karlsruhe Light Technology Institute, Germany	*Ferroelectricity in Perovskite Solar Cells*
16	Dec 15	**Ahmad Safari**	School of Engineering, Rutgers University, New Jersey	*Piezoelectric and Dielectric Composites*

FAU-NITech Lecture Series

The original plan for this interdisciplinary graduate level lecture series was that each module, including a course held by both a FAU PI and a NITech PI, is grouped into one-week block modules. Unfortunately, this compact format, and the exchange of PIs between Germany and Japan was not possible.
However, all six PIs made an effort to make the lectures available online by filming and exchanging their course materials.

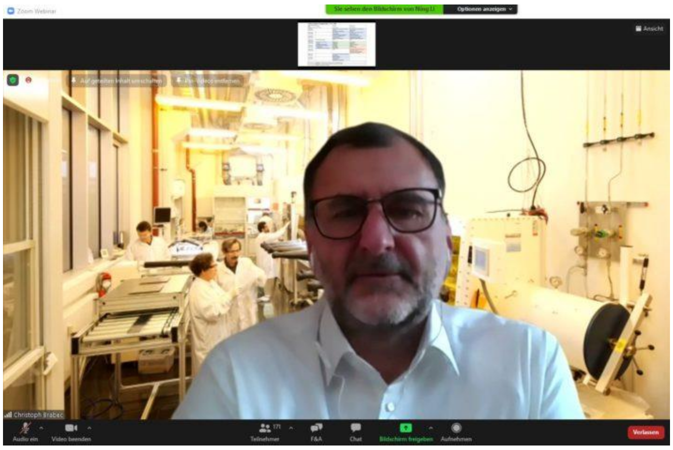
The size of the modules (5 ECTS) fit seamlessly into the academic programs of 10 master courses at FAU and there have been more than ten MSc students external to the IRTG who one of our joined our lectures.

This year, this series consists of introductory lectures focused on lead-free ferroelectrics, materials and devices for optoelectrics, and modeling techniques, and each doctoral researcher is expected to join one module.

	Title	Lecturer
1	**Introduction to atomistic and mesoscale modeling**	
	1. Electro-Mechanical-Modeling (EMM)	Prof. Paul Steinmann
	2. Simulation for Nano-Technology	Prof. Shuji Ogata
2	**Introduction to lead-free perovskite ferroelectrics for electro-mechanical systems**	
	1. Electromechanical Properties of Ferroelectrics	Prof. Kyle G. Webber
	2. Piezoelectric Properties of Lead-Free Ferroelectrics	Prof. Ken-ichi Kakimoto
3	**Materials and devices for opto-electric and energy technologies**	
	1. Next Generation Solar Energy (NGSE5)	Prof. Christoph Brabec
	2. Electronic Materials Analysis	Prof. Kato

International Conference on Next Generation Solar Energy (NGSE5)

The IRTG was a partner of the fifth International Conference on Next Generation Solar Energy (NGSE5) held from 7th – 9th of December 2020. The conference concept introduces the topic “Next Generation Solar Energy” with a series of 50 min tutorials. A series of 15 min long impulse lectures on current results and trends complements the concept. The conference offered an excellent opportunity to learn about latest developments and current projects in the field of organic and perovskite photovoltaic technology.



Prof. Brabec presenting the NGSE5 Schedule to the participants

Collaborative Project Progress Report Presentations (October 7th)
The Kick-off meeting marked the beginning of the Collaborative Research Project on Integrated Coupled Energy Harvesting Systems, where four teams of our doctoral researchers at FAU and NITech work collaboratively to address the scientific question: “How can the electro-optical (photovoltaic) and electro-mechanical phenomena be coupled into one system?”

After working on their research concepts for six month, they presented their initial findings and results. The final presentations will be held at the FAU-NITech School on Energy Systems in March 2021, where the winning team will be announced.

Team 1 “Investigation of stress-dependent material properties of Energy Harvesters”

Juliana Maier (F), Andreas Hegendörfer (C), Christian Kupfer (E), Ismail Haque (A)

Team 3 “In Depth Examination of Photostriction in Lead-Free Perovskites”

Tim Freund (I), David Köllner (D), Yuta Yamamoto (G)

Team 2 “Electrooptical and Electromechanical Coupling of Photoferroic Solar Cells”

Ahmed Gadelmawla (H), Viktor Rehm (J), Samuele Spreafico (L), Choi Min Uk (E)

Team 4 “Tailoring the conversion of a multilayered material with nano piezoelectric and phototronic effects”

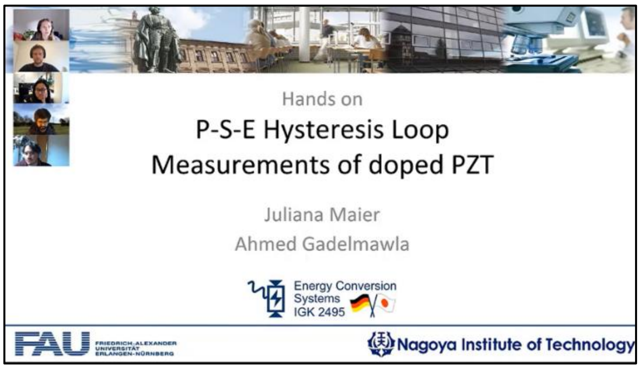
Gabriel Stankiewicz (B), David Dobesh (G), Niharika Gogoi (A), Takahiro Tsuzuki (K)

Tutorials and Hands-on Workshops

The session of tutorials and hands-on workshop, which were supposed to be offered at the Yearly Schools in 2021 and 2022, has undergone profound change due to the pandemic. At present, one of 12 tutorials, each coupled with a workshop, will be presented every month in 2021.

Through the tutorials, the doctoral researchers will learn more in-depth information about a particular aspect of materials development, synthesis, simulations, or devices. In addition, the hands-on workshops organized by doctoral researchers will give a hands-on experience with various techniques.

In December, Prof. Kyle Webber (Project F and H) and doctoral researchers Juliana Maier (Project F) and Ahmed Gadelmawla (Project H) marked the beginning of the session, and showed how it is possible to offer a hands-on workshop virtually.



Online "Hands-on" Workshop by Juliana Maier and Ahmed Gadelmawla

Intercultural Training

To prepare FAU doctoral researchers for extended research visits in Japan, but also to make all members aware of cultural differences, the IRTG works closely with the Japanese Studies Institute, FAU. We have adapted the program to the travel restrictions and have presented an Info Session about “Tips for the Online Communication with Japanese Colleagues" this year in August. The program will be continued in 2021. Vice versa, NITech offered an Intercultural Seminar for their doctoral researchers including intensive English training, risk management for overseas travel, and information on German culture and living in Germany.

3.2. Research Stays or internships at other institutes

Ahmed Gadelmawla

From / to	Institute visited	Local Supervisors	research activities performed and skills acquired
09.-13.03.20	University Bremen	Dr. Johannes Birkenstock	HTK-XRD

Jonas Biggemann

From / to	Institute visited	Local Supervisors	research activities performed and skills acquired
02.03.20	Caltech, Pasadena, CA, USA	Prof. K. Faber	Oral presentation of the Department of Applied Physics and Material Science: ”Modular Ceramic Building Block Composites for Biomedical Applications”

3.2.1. Research Stays at the respective partner institute

From / to	Institute visited	Local Supervisors	research activities performed and skills acquired
10.-21.02.20	SPring-8 and NITech	Prof. Koichi Hayashi	XFH

The difference between NITech and FAU was not that much as I expected. Actually, there were minor differences due to the culture and in the system. For example, most of the student assistants there were bachelor students. The number of master students and PhDs is not comparable to what we have in FAU. That could be due to the high education fees. I have not noticed many international students. The students there show high respect for ranking and teachers. Titles in Japan are really a big thing. You always have to be careful with whom you talk to and give him his appropriate title like [sensei, san, kun]. The mensa system is almost the same idea as in FAU but with wide varieties, but unfortunately, everything there is in Japanese, and it is rare to find words in English. The communication was not easy because of the language barrier.

Generally, people there are friendly, helpful, workaholic (e.g., about 12 hours a day), hospitable, and modest. I love that when we go together to the mensa as a team and work together also as a team. During the experiments, everyone work with hands. No one can tell the difference between professor, postdoc, or normal workers. Nagoya as a city is enriched with cultural places to visit. I was so lucky to find some free time to visit Nagoya castle. The transportation system is totally different than in Germany. I struggled to navigate and pay for the tickets, as you have to pay with a chargeable card called ICOCA. You always have to keep cash with you because they do not use cards frequently.

In summary of my experience, the people, the food, the country, and the university are great. Nevertheless, there were difficulties in communication due to the language barriers. However, people were super friendly and tried to help me as much as possible by using gestures to explain. I differently will go there again not only for work but to enjoy the country.

Ahmed Gadelmawla

3.3. Gender Equality

Workshops and seminars

Together with the RTG2423 FRASCAL “Fractures Across Scale” the “Understanding Gender” Module Series with three modules in 2020 was organized to sensitize doctoral researchers for aspects of gender in the context of research and science.

	Date	Title	Lecturer
1	30.04.20	Understanding Gender This workshop provided a brief introduction to how gender plays a role in everyday life at the university.	Dr. Frölich-Steffen
2	30.10.20	Gender Competence Training In this workshop participants were introduced to “gender competence” in their research and teaching areas.	Dr. Sabine Blackmore
3	20.11.20	Gender in Teaching and Learning This workshop aimed to expand the gender perspective and skills of teachers at university.	Dr. Frölich-Steffen

First Gender Seminar

The IRTG is a member of the Research Associations of Friedrich-Alexander-University Erlangen-Nürnberg for the promotion of equality (F3G). They organize workshops that also the IRTG members could participate.

	Date	Title	Lecturer
1	18.05.20	Self-Presentation	Julia Baumeister
2	29.05.20, 22.06.20	Time Management	Peter Kronenberg
3	23.10.20, 26.10.20	Publishing in Science, Technology, Engineering and Medicine	Team of the FAU Library

Further measures

The IRTG has purchased two cuby boxes that can be used freely at the institutes LTM or Glass and Ceramics, and we have contributed to the F3G coordination costs. Flexible working hours enable a good work-life-balance.

3.4. Meetings

IRTG-Director Prof. Kyle Webber and Coordinator Julia Berger met with the doctoral researchers every three month. Since August, project presentations by the PhD students have been included. In 2021, meetings will be held more regularly and NITech members will be included more.

4. Appendices

4.1. Program Kick-off Meeting

4.2. Program Collaborative Project Progress Presentations

4.3. List of book inventory

4.1. Program Kick-off Meeting

Date: February 24th – 26th 2020		
Venue: Residenzschloss Hotel, Bamberg		
Program Day 1		
09:45 – 10:15	Opening and Welcome by Prof. Kyle G. Webber and Prof. Ken-ichi Kakimoto	
10:15 – 11:00	Project Group Discussions	
11:00 – 12:00	*Lunch Break*	
12:00 – 13:00	Presentations by Industrial Advisors Dr. Gunnar Picht (Robert Bosch GmbH) Dr. Oliver Schmidt (Siemens AG)	
13:15 – 17:45	Project Presentations, presented by PIs	
18:45	*Joint Dinner*	
Program Day 2		
08:30 – 11:30	Ring Lectures by	Prof. Georg Fischer Dr. Julia Mergheim Dr. Tobias Fey Prof. Paul Steinmann
11:30 – 12:30	*Lunch Break*	
12:30 – 15:00	Ring Lectures by	Dr. Rita Cicconi Prof. Peter Wellmann Prof. Christoph Brabec
15:30 – 18:30	PI Meeting and Workshop “Good Scientific Practice” by Dr. Christian Schmitt-Engel (FAU)	
18:30	*Joint Dinner*	
Program Day 3		
08:30 – 11:00	Ring Lectures by	Prof. Kyle Webber Prof. Wolfgang Heiss Dr. Wendler Prof. Bernd Meyer
11:30 – 12:00	Concluding Remarks	
12:00 – 15:30	Cultural Program	

4.2. Program Collaborative Project Progress Presentations

Date: October 7th 2020	
Venue: H14 in Martensstraße 5, Erlangen	
09:00 – 09:15	Opening and Welcome by Prof. Kyle G. Webber
09:15 – 09:45	Group 1: Investigation of stress-dependent material properties of Energy Harvesters
09:45 – 10:15	Group 2: Electrooptical and Electromechanical Coupling of Photoferroic Solar Cells
10:15 – 10:45	Group 3: In Depth Examination of Photostriction in Lead Free Perovskites
10:45 – 11:15	Group 4: Tailoring the conversion of a multilayered material with nano piezoelectric and phototronic effects
11:15	Joint Lunch

4.3. List of book inventory

	Author	Title	Publishing Year
1	Jean-Paul Pelteret and Paul Steinmann	Magneto-Active Polymers	2019
2	Sasaki Yuji	3D Local Structure and Functionality Design of Materials	2019
3	Vegas Molina	Structural Models of Inorganic Crystals: from the Elements to the Compounds	2018
4	Pozar, David M.	Microwave Engineering	2011
5	Richard J. D. Tilley	Perovskites: Structure-Property Relationships	2016
6	Markys G. Cain	Characterisation of Ferroelectric Bulk Materials and Thin Films	2014
7	Peter Schaaf	Laser Processing of Materials	2012
8	Eric R. Scerri	The Periodic Table. Its Story and Its Significance	2006
9	Govindhan Dhanaraj, Kullaiah Byrappa, Vishwanath Prasad, Michael Dudley	Springer Handbook of Crystal Growth	2010
10	Tze-Chien Sum, Nripan Mathews	Halide Perovskites: Photovoltaics, Light Emitting Devices, and Beyond	2019
11	Patricia Gosling	Mastering your PhD	2006
12	Peter W. Atkins	Molecular Quantum Mechanics	2010
13	Markys G. Chain	Characterisation of Ferroelectric Bulk Material	2014