Annual Report 2022

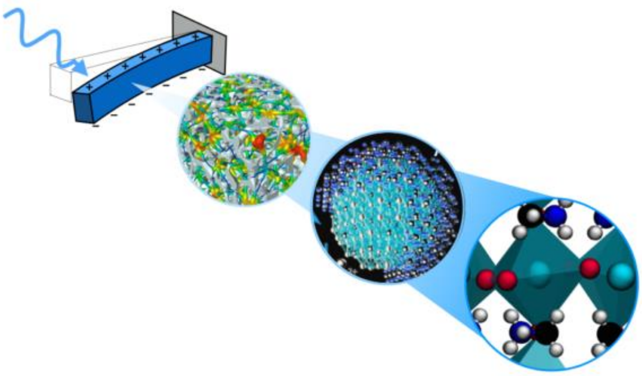
of the International Research Training Group GRK 2495

in collaboration with Nagoya Institute of Technology (NITech)

Director: Prof. Dr. Kyle Webber

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

Energy Conversion Systems IGK 2495



First funding period: 01.12.2020 – 30.06.2024

Impressum

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91058 Erlangen
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julia.b.berger@fau.de

Preface

This year was marked by the official end of the pandemic in many parts of the world, meaning that borders opened up, masks came off, and people were more easily able to meet again. Despite Corona not disappearing completely and many people still being significantly impacted by its effects, these important developments began to return some level of normalcy. For the IRTG, this was also the first time since 2020 that open travel between Germany and Japan was allowed, which we utilized to send a large group of researchers to Nagoya in the late summer as soon as visas were possible. The effects on the doctoral researchers as well as the IRTG as a whole were dramatic and immediate in terms of research collaborations, communication, and research goals.

With our eyes toward the future, we will be building upon these positive developments in 2023 and beyond, with increased academic exchanges and cultural events between FAU and NITech as well as training and social events at FAU. This will begin with the Kick-Off Meeting that will be held at Gifu, Japan in late February 2023. And, very importantly, we will be officially welcoming our second generation of FAU doctoral researchers to the team in January 2023!

It is a very exciting time in the IRTG and we all look forward to continued international collaboration and partnership between NITech and FAU!

Prof. Dr. Kyle G. Webber

Efforts to accept IRTG students and dispatch JGGE students abroad had been severely affected by global travel restrictions due to the new coronavirus infection. However, due to new measures taken by the Japanese government and national universities since May 2022, mutual dispatches have finally resumed. At NITech, cross-cultural exchanges with FAU students were further promoted, English communication became the norm, and younger students were able to feel closer to the significance and fun of studying abroad in the future.

Traditional international exchange through face-to-face encounters between people, has now reached a major turning point, having experienced remote education system via the Internet in the age of With Corona. However, as an old saying goes, "To see a friend from far is a joy." Studying abroad, in which students actually visit another place to learn, has great values in understanding different cultures and building diverse human networks through exchange activities outside of working or study hours.

In year 2023, the second group IRTG students will play a leading role in international exchange between FAU and NITech. We hope to further deepen international exchange and education/research by taking many advantages experienced by the first group of students.

Prof. Dr. Ken-ichi Kakimoto

Content

1. General Information
1.1. Participating Researchers

Table 1a: Participating FAU Principal Investigators

Principal Investigators	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, PD 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, 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

Table 2b: Participating NITech Principal Investigators

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 3a: Participating FAU Doctoral Researchers

Doctoral Researchers	**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
Durdiev, Dilshod	Materials Simulation, Dep. of Materials Science and Engineering, Dr.-Mack-Str. 77, 90762 Fürth	+49 911 65078-65065 dilshod.durdiev@fau.de http://www.matsim.techfak.uni-erlangen.de	Phase Field Modeling
Gadelmawla, 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
Hegendörfer, 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.dehttps://chemistry.nat.fau.eu/	Computational Chemistry
Stankiewicz, 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
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

Table 4b: Participating NITech Doctoral Researchers

Dmitrieva, Daria	Frontier Research Institute for Information Science, Dep. of Electrical and Mechanical Engineering, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan	evh89634@ict.nitech.ac.jp	Wearable Communication Devices
Duan, Xianyi	Dep. Of Electrical and Mechanical Engineering, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan	x.duan.505@nitech.jp	Bioelectro-magnetic, Electromagnetic
Gan, Rongguang	Advanced Ceramics Research Center, Dep. of Life Science and Applied Chemistry, 10-6-29 Asahigaoka, Tajimi, Gifu 507-0071, Japan	r.gan.311@stn.nitech.ac.jp	Heterogeneous Catalysts
Haque, Md Ismail	Dep. Of Electrical and Mechanical Engineering, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan	ismaileeeruetpg@gmail.com	Human body communication
Kongshik, Rho	Frontier Research Institute for Material Science, Dep. of Electrical and Mechanical Engineering, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan	k.rho.991@stn.nitech.ac.jp	Characterization of 3C-SiC as photocatalys
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
Otsuka, Takahito	Frontier Research Institute for Material Science, Dep. of Life Science and Applied Chemistry, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan	t.otsuka.098@stn.nitech.ac.jp	Optical Materials
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, Ryota	Frontier Research Institute for Material Science, Dep. of Life Science and Applied Chemistry, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan	r.yamamoto.414@stn.nitech.ac.jp	Electronic Ceramics
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
Zhang, Endong	Frontier Research Institute for Material Science, Dep. of Electrical and Mechanical Engineering, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan	e.zhang.635@stn.nitech.ac.jp	Characterization of Energy Conversion Materials

Table 5a: Participating FAU and NITech Associated Researchers and Post-Doctoral Researchers

Associated Researchers/ Post Docs	Chair, Department, Address	Tel/ Fax, Email, Web	Research Area
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
Hoffmann, Patrizia	Glass and Ceramics, Dep. of Materials Science and Engineering, Martensstr. 5, 91058 Erlangen	+49 9131-8527540 patrizia.hoffmann@fau.de http://www.glass-ceramics.uni-erlangen.de	Cellular Ceramics and Simulation
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
Shi, Xi, Dr.	Glass and Ceramics, Dep. of Materials Science and Engineering, Martensstr. 5, 91058 Erlangen	+49 9131-8527540 xi.shi@fau.de http://www.glass-ceramics.uni-erlangen.de	Mechanical and Energy Storage Properties of Antiferroelectric Ceramics
Swantje, Simon	Glass and Ceramics, Dep. of Materials Science and Engineering, Martensstr. 5, 91058 Erlangen	+49 9131-8527540 swantje.simon@fau.de http://www.glass-ceramics.uni-erlangen.de	Cellular Ceramics and Simulation
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
Tshikwand, Georgino	Materials Simulation, Dep. of Materials Science and Engineering, Dr.-Mack-Str. 77, 90762 Fürth	+49 911 65078 65064 georgino.tshikwand@fau.de http://www.matsim.techfak.uni-erlangen.de/	Coupled Finite Element Simulation of Shape Memory Alloys
Ziegler, Andreas	Computer Chemistry Center. Dep. of Chemistry and Pharmacy, Nägelsbachstr. 25, 91052 Erlangen	+49 9131 8520424 andreas.az.ziegler@fau.de https://www.chemistry.nat.fau.eu /icmm/	Computational Chemistry
Anzai, Daisuke, Dr.	Frontier Research Institute for Information Science, Dep. of Electrical and Mechanical Engineering, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan	anzai.daisuke@nitech.ac.jp	Wearable Communication Devices
Gomez-Tames, Jose, Dr.	Frontier Research Institute for Information Science, Dep. of Electrical and Mechanical Engineering, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan	gomeztames.josedavid @nitech.ac.jp	Bioelectro-magnetics
Ishii, Yosuke, Dr.	Graduate School of Engineering, Dep. of Physical Science and Engineering, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan	ishii.yosuke@nitech.ac.jp	Nanocarbon chemistry
Kimura, Koji, Dr.	Frontier Research Institute for Information Science, Dep. of Electrical and	kimura.koji@nitech.ac.jp	X-ray characterization

	Mechanical Engineering, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan		
Kobayashi, Ryo, Dr.	Graduate School of Engineering, Dep. of Physical Science and Engineering, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan	kobayashi.ryo@nitech.ac.jp	Multiscale computer simulation of materials
Nishida, Yoshihide, Dr.	Advanced Ceramics Research Center, Dep. of Life Science and Applied Chemistry, 10-6-29 Asahigaoka, Tajimi, Gifu 507-0071, Japan	nishida.yoshihide@nitech.ac.jp	Heterogeneous Catalysts
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
Uranagase, Masayuki, Dr.	Graduate School of Engineering, Dep. of Physical Science and Engineering, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan	uranagase.masayuki@nitech.ac.jp	Multiscale computer simulation of materials
Urushihara, Daisuke, Dr.	Frontier Research Institute for Information Science, Dep. of Electrical and Mechanical Engineering, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan	urushihara.daisuke@nitech.ac.jp	Electronic Ceramics

Table 6: Student Assistants

Students Assistants	**Project, Supervisor**	**Research Area**	**Member (from – to)**
Almaabri, Osamah	Project F, Juliana Maier	Nanotechnology	Mar 2022–Sep 2022
Banerjee, Semanti	Project H, Ahmed Gadelmawla	Materials Science	Jan 2022–Aug 2022
Chandramouli, Nikhil	Project B, Chaitanya Dev	Computational Engineering	Apr 2021–Mar 2022
Eyoum, Gina	Project H, Kyle Webber	Functional Ceramics	Since May 2020
Fuggerer, Tim	Project F, Juliana Maier	Nanotechnology	Apr 2021–Mar 2022
Guo, Han	Project I, Peter Wellmann	Nanotechnology	Since Sep 2022
Kraft, Viktoria	Project H, Kyle Webber	Materials Science	Nov 2022–Dec 2022
Monavvar, Milad	Project I, Tim Freund	Computational Engineering	Since Nov 2021
Papadaki, Anastasia	Project K, Dilshod Durdiev	Computational Engineering	Nov 2021–Jan 2022
Qin, Yuchin	Project A, Niharika Gogoi	EEI	Oct 2021–Jan 2022
Shu, Huan	Project J, Wolfgang Heiss	Materials Science	Nov 2021–Mar 2022
Sell, Marlene	Project L, Bernd Meyer	Chemistry	Jun 2022–Sep 2022
Spath, Isabella	Project D, Tobias Fey	Nanotechnology	Since Apr 2021
Vo, Nadia	Project G, Rita Cicconi	Nanotechnology	Since Aug 2020
Wolf, Edwyn	Project D, David Köllner	Materials Science	Since Jun 2021
Xiao, Keyu	Project A, Niharika Gogoi	Medical Engineering	Sep 2022–Dec 2022
Yaser, Abdallah	Project A, Niharika Gogoi	EEI	Oct 2021–Apr 2022
Zhang, Jianqi	Project J, Wolfgang Heiss	Materials Science	Since Oct 2022
Zücklein, Julian	Project I, Peter Wellmann	Materials Science	Since Feb 2022

Table 7: Industrial Advisors

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

Table 8: Project Coordination and Administration

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
Kawamura, Ayuko	Nagoya Institute of Technology	+81 52735-5193, ayuko.kawamura@nitech.ac.jp jgge-secretaiat@adm.nitech.ac.jp	Assistant Administrative Staff

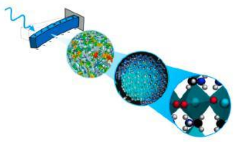
1.2. Reporting Period

01 January 2022 to 31 December 2022

Info Flyer

Qualification Program

A variety of interdisciplinary, theoretical, and practical training with integrated soft skills training is offered to the Doctoral Researchers. They get direct access to a wealth of collaboration opportunities, new scientific concepts, practical experience, cutting-edge experimental equipment and simulation methods, and international experts and industrial partners.



Completion in three years

Year 1
- Kick-off Meeting
- Ring Lectures
- Introductory Lecture Series
- Collaborative Project
- Invited Colloquia
- Soft Skill Workshops

Year 2
- 1st IRTG Yearly School
- Tutorials and Hands-on Workshops
- Focused Lecture Series
- Collaborative Project
- Invited Colloquia
- Japanese Cultural Program
- Soft Skill Workshops

Year 3
- 2nd IRTG Yearly School
- Tutorials and Hands-on Workshops
- Advanced Lecture Series
- Invited Colloquia

Contact:

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Friedrich-Alexander-University
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Martensstraße 5, 91058 Erlangen
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Nagoya Institute of Technology
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Gokiso-cho, Showa-ku, Nagoya 466-8555
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julia.b.berger@fau.de

FRIEDRICH-ALEXANDER
UNIVERSITÄT
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International Research Training Group
GRK 2495:

ENERGY CONVERSION SYSTEMS
From Materials to Devices

Energy Conversion Systems IGK 2495

Research Program

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

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

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

Project D Additive Manufacturing of Cellular Lead-Free Ceramics

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

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

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

Project H Stress Modulated Electromechanical Coupling of Lead-Free Ferroelectrics

Project I Growth of Single Crystal Transition Metal Perovskite Chalcogenides

Project J Solution Processed Ferroelectrics in Photovoltaic Devices

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

Project L Modeling of Defect and Surface Chemistry of Perovskites

We aim to create an international learning lab to train the next generation of scientists and engineers to work on sustainable energy solutions. Perovskite materials show significant promise for energy applications including energy conversion and storage for cutting edge applications.

Nagoya Institute of Technology

The IRTG is specifically designed to bring together scientists and research groups from Germany and Japan with complementary expertise to facilitate internal and international collaboration.

NITech and FAU are departmental partners since 2009, and University level partners since 2011. The GRK 2495 will strengthen this partnership.

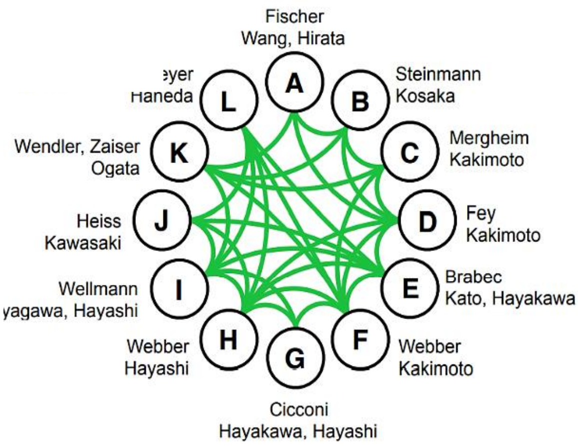
Our partner institute NITech is located in Nagoya, in the Aichi prefecture. Aichi is located in the center of Japan, and is known as the center of Japanese technology. You can find a wide range from traditional industries like ceramics to cutting edge industries like automobiles.

JAPAN SOCIETY FOR THE PROMOTION OF SCIENCE
日本学術振興会

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

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

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

Objectives and status

The project is inspired by smart shoe design. The walking and running activity is a source of mechanical energy, which can excite piezos to generate energy. Taking the advantage of this possibility, we aim to integrate piezos in a shoe inlay to harvest energy and acquire sensor data from foot movement. This opens up avenues for ambient energy harvesting and wearable shoe sensors for health monitoring, medical diagnosis and sports training. The main aim of our project is to design an electronic circuit, which can maximize the usable energy generated from the feet movement. The electronic circuit will be optimized with maximum power point tracking and synchronous switch harvesting circuit.

We divided the project into following sections, which are elaborately discussed below:

- Electrical Modelling: An electrical equivalent model is important to understand the electrical behaviour of the ceramics. We take two approaches to derive the model. At first, we design an electrical model by impedance analysis and secondly we derive the model via Finite element analysis. The second approach is in association with Project C and in this approach, we aim to relate the mechanical and electrical parameters. Status: Completed
- Human Gait Acquisition Circuit: The gait pattern and waveform of generated energy is expected to share a correlation. Therefore, we design a human gait acquisition circuit is to know the gait pattern of the foot movement. Status: Completed
- Electronic Circuitry: The electronic circuitry is responsible to convert the uncertain electrical power generation into constant supply of power output. Now we are focussing on advanced circuitry to increase the overall efficiency of the system. Status: Completed
- Shoe layout design: Although our primary focus is circuit advancement, a proper shoe layout design is also important for us when we want to take full advantage of energy harvest from walking or running. Initially, we did not take the shoe structure with integrated piezo arrays into consideration, which resulted in lot of power absorption by the sole itself. Now, the layout design is taken into account as important as the circuitry. Status : Completed

Conclusions, main achievements and outlook

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.

This work is based on implementing piezoelectric elements as sensors and energy harvesters. The objectives set in the beginning of research study has been achieved in the last 3 years. A comfortable shoe sole design has been proposed with electronic circuits integrated for sensing and energy harvesting. The total harvested energy from walking have successfully helped in operating the sensing unit for UART connection without relying on a battery. However, for Bluetooth data transmission, as the power demand is much higher than multiple piezoelectric elements can generate, the system fails to operate without battery.

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.

The electrical modeling mentioned in section 1 was fundamental point to start with our circuit simulation. In addition, human gait acquisition was important to understand the pressure map on the foot, which is directly related to the energy generated by walking/running. We mimic the observation from gait signals to generate similar input to the derived model for system level simulation. This preliminary study helped us to design our energy harvesting circuitry, which have been experimentally tested.

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. Unfortunately, the piezoelectric elements provided could not be connected with any wire. This made it difficult to integrate in our circuit due to connection issues.

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 and Takeshi Okada

Objectives and status

The objective of this work is to develop a computational framework to design mechanical structures using topology and shape optimization. The developed methodology should be integrated into an open source code, based on the finite element method library deal.II. Primary applications of the software are the design of shape adaptive structures (compliant mechanisms) that undergo large deformations and piezoelectric structures in which maximization of piezoelectric coefficients is the objective.

Currently, the software supports:

- Novel coupling approach for topology and shape optimization using embedding domain discretization (EDD) method. The coupling is implemented in linear elasticity setting in 2D.
- Topology and shape optimization of compliant mechanisms in linear and nonlinear elasticity setting in 2D. Additionally, Von Mises stress constraints and various manufacturing constraints, for instance a curvature constraint, are implemented in shape optimization to ensure feasibility of the obtained final shapes of the structures, see Fig. 1.
- Shape optimization for maximization of electromechanical coupling coefficient for bimorph piezoelectric energy harvesters in 3D.
- Computational homogenization of piezoelectric periodic structures in both standard and EDD setting.
- Topology optimization of dynamic vibration absorbers considering the natural frequency constraint.
- Simulation of interfaces between two orthotropic materials in EDD setting.

In the next phase of the project the following functionality will be implemented:

- Shape optimization of piezoelectric periodic structures for maximization of their respective material coefficients, e.g. hydrostatic piezoelectric coefficient. Computational homogenization will be utilized to compute the effective material properties of the structures in each optimization iteration
- Shape optimization of interfaces between two solid materials for maximal stiffness and interface stresses.

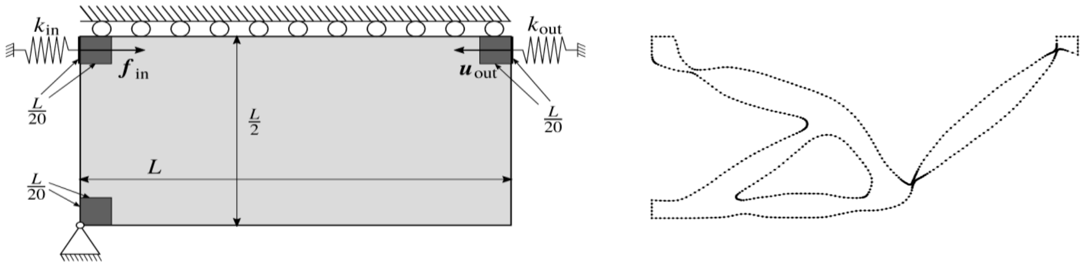


Figure 1: Left image: Design setup for the design of compliant mechanism (displacement inverter) using topology and shape optimization. Right image: Obtained shape, displayed using nodal design variables.

Until now, structural optimization of piezoelectric periodic structures is limited to rough topology optimization in which the information about exact boundary is lacking [1]. Similarly, structural optimization of material interfaces has been explored by means of topology optimization or shape optimization in the level set method framework [2]. No implementation, however, in the node-based shape optimization setting is available in the literature.

Conclusions, main achievements and outlook

The outcome of the work of the researchers from project B is an advanced, open source C++ software based in deal.II library that supports various of applications of combined topology and shape optimization including; the design of shape adaptive structures (compliant mechanisms) in linear and nonlinear elasticity setting using stress and curvature constraints; computational homogenization of periodic piezoelectric structures, simulation of material interfaces, topology optimization of dynamic vibration absorbers and novel coupling approach for topology and shape optimization.

The novel coupling approach for topology and shape optimization has been presented online at *International Conference on Adaptive Modeling and Simulation (ADMOS)* in Göteborg, Sweden, 2021 and at *16th U.S. National Congress on Computational Mechanics* in Chicago, USA, 2021. The results of this work have been summarized in a journal article. Additionally, the work on topology and shape optimization of compliant mechanisms using stress and curvature constraints have been published in two journal articles. Those articles are listed in section 3.

The work on computational homogenization of periodic piezoelectric structures was performed after discussions with the members of Project D for the auxetic cells of their interest. Furthermore, the methodology for the topology optimization of dynamic vibration absorbers was developed for the specific application of a stator of an electric motor, vibration suppression of which is the main the focus of the work of Project B at NITech.

[1] Sigmund, Ole, Salvatore Torquato, and Ilhan A. Aksay. "On the design of 1–3 piezocomposites using topology optimization." Journal of materials research 13.4 (1998): 1038-1048.

[2] Najafi, Ahmad R., et al. "A gradient-based shape optimization scheme using an interface-enriched generalized FEM." Computer Methods in Applied Mechanics and Engineering 296 (2015): 1-17.

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 and Ryota Yamamoto

Objectives and status

A piezoelectric vibration-based energy harvester (PVEH) is a combined device consisting of an electromechanical structure in conjunction with an electric circuit. Such a device converts ambient vibration energy into electric energy to drive low-power electronics. The piezoelectric effect is an interaction between mechanical and electrical quantities and is exploited as the energy conversion mechanism of PVEHs. Simulations and optimizations of PVEHs facilitate rapid development and increase their efficiency. In addition, novel piezoelectric composite materials extend the application range of PVEHs to high temperature environments.

In collaboration with NITech, a synthesis of a novel piezoelectric composite material composed of polyimide and (Na,K)NbO_3 (PI/NKN) is carried out in [1]. By applying mechanical vibration and heat, the frequency and output voltage of the new composite material are investigated from room temperature up to 200°C. The measurements show that the key parameters, namely piezoelectric constant and relative permittivity, exhibit excellent high-temperature stability. Therefore, PI/NKN composites are potential energy harvesting materials suitable for PVEHs operating in high temperature environments.

In [2] an implicit coupling between a finite element method (FEM) simulation of the electromechanical structure and an electronic circuit simulator (ECS) for the analysis of the electric circuit is introduced. The advantage of the implicit coupling method is, that the full capabilities of the FEM can be exploited without restrictions for accurate simulations of nonlinear electromechanical structures. Furthermore, using an ECS allows for the consideration of arbitrary electric circuits, resulting in highly realistic simulations of PVEHs. No simplifications are introduced in the coupling method, meaning that arbitrary PVEHs can be analyzed. Figure 1 presents the electrode voltage φ_{el} of a shock excited PVEH with a practical self-powered synchronized switch harvesting on inductor (SSHI) circuit. In the beginning of the simulation the oscillation of the electrode voltage φ_{el} is superimposed by higher frequency modes. After around 30ms these higher frequency modes are decayed and the oscillation is mainly limited to the first vibration mode. The interaction between the SSHI circuit and the electromechanical structure is precisely considered. This example demonstrates the practical applicability of the novel coupling method for realistic simulations of PVEHs.

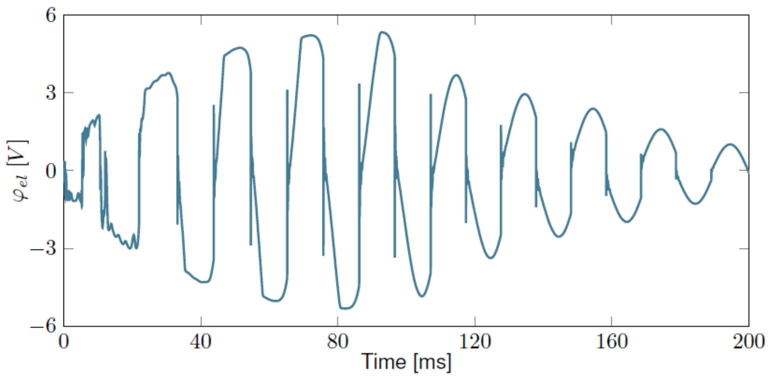


Figure 2: Electrode voltage φ_{el} of a nonlinear electromechanical structure coupled to a practical self-powered SSHI circuit as a response to a shock base-excitation.

In [3] the harvested energy of a PVEH is maximized taking into account a nonlinear stress constraint. In the optimization problem, a bimorph electromechanical structure equipped with the Greinacher circuit and the standard circuit is considered and different electrical and mechanical design parameters are introduced. Using the implicit FEM-ECS coupling method, deep neural network (DNN) training data are generated, allowing for a computationally efficient evaluation of the objective function. Subsequently, a genetic algorithm using the DNNs is applied to find the optimal parameter values of the PEH and the results are carefully analyzed.

Conclusions, main achievements and outlook

In collaboration with NITech, a novel piezoelectric PI/NKN composite material was investigated. Due to its excellent temperature stability, this material potentially expands the application range of PVEHs to high temperature environments.

Moreover, a novel implicit FEM-ECS coupling method has been introduced, which overcomes all limitations of monolithic and explicit FEM-ECS couplings reported in the literature. The practical applicability of the coupling method for the simulation of realistic PVEHs is demonstrated. As a result, the novel simulation method can be used to reduce experimental effort and cost in the development process of PVEHs.

Subsequently, a PVEH consisting of different electric circuits and a bimorph electromechanical structure has been optimized taking into account a nonlinear stress constraint. To avoid high computational effort during the optimization procedure a DNN was trained. The results show that due to the piezoelectric effect the optimal electric circuit parameters depend on the mechanical parameters and vice versa. Using the proposed optimization procedure optimal electrical and mechanical parameters of a PVEH can be found increasing the efficiency of PVEHs.

[1] Yamamoto et al. "Temperature-dependent vibration energy harvesting performance of polyimide/(Na, K) NbO3 piezoelectric composites." Japanese Journal of Applied Physics 61.SN (2022): SN1028.

[2] Hegendörfer et al. “An implicitly coupled finite element - electronic circuit simulator method for efficient system simulations of piezoelectric energy harvesters.” Journal of Intelligent Materials Systems and Structures.

[3] Hegendörfer et al. “Numerical optimization of a nonlinear nonideal piezoelectric energy harvester using deep learning.” Journal of Low Power Electronics and Applications.

D – Additive Manufacturing of Cellular Lead-Free Ceramics

FAU: Tobias Fey, David Köllner, Swantje Simon and Patricia Hoffmann
NITech: Ken-ichi Kakimoto

Objectives and status

This work aims to fabricate cellular lead-free ceramics via additive manufacturing and to investigate the structural, mechanical, and piezoelectric properties. The focus is on correlating the different properties to improve sensor, actuator, and energy harvesting applications. In the third year, the manufactured $(BaCa)(ZrTi)O_3$ (BCZT) honeycomb unit cells with a varying structural angel (-35° to 35°) were characterized and compared to a FEM simulation. The results of the mechanical properties proved previous observations of alumina honeycombs. A correlation between structural parameters and piezoelectric properties was also established. It is now possible to produce cellular structures with high piezoelectric constants and high mechanical strengths, which are clearly superior to conventional piezoelectric foams. In addition, open-celled ceramic honeycombs were fabricated via a combination of stereolithography and replica techniques. Despite the increased porosity, very promising initial results were obtained, such as high piezoelectric coefficients. In the future, further piezoelectric measurements (Polarisation-Strain-Electric field Loops) must now be performed to better understand the relationship between cellular structure and properties, and the difference between indirect and direct excitation.

Conclusions, main achievements and outlook

The third year concentrated on the mechanical and piezoelectric characterization of BCZT honeycombs with angles between -35° and 35°. These were manufactured from the BCZT powder from NITech via injection molding. The mechanical properties were determined via compression test and DIC, partly shown in Figure **2**. The compressive strength depends strongly on the angle and is a minimum of 0.91 MPa at 30° and a maximum of 94.60 MPa at 0°. As already shown on alumina, the good agreement of these values with the model of Gibson and Ashby is confirmed. However, this does not apply to the Poisson's ratios. Here, the measured values deviate from the model. Nevertheless, a FEM simulation could be carried out, in which a good agreement with the measurements is achieved. In contrast to the Gibson and Ashby model, the Young's modulus and the overall dimensions are included in the FEM calculation. A minimum Poisson's ratio was found at -20° of -2.17 and a maximum at 15° of 1.52. Based on the mechanical properties, it can be seen how great the potential for modification of the honeycombs is. The piezoelectric properties were determined by the Berlincourt method and also show a dependence on the structural angle. The d_{33} is between 180 and 296 pC/N, which means that the cellular structures even exceed the dense references (d_{33} = 191 pC/N) by a factor of 1.5. Whereas no clear trend can be seen for the d_{33}, the g_{33} increases linearly with increasing angle from -35 to +35°. The g_{33} values of the honeycombs (-30°, 0.07 Vm/N) exceed those of the references (0.01 Vm/N). It could be observed that this is due to the porosity but also to the structure, which on the one hand, allows good polarization, and on the other hand, has higher surface stresses, as determined by FEM simulations.

Through a combination of replica process and stereolithography, more complex 3-dimensional cellular structures could be fabricated from alumina, barium titanate, and BCZT. Mechanically, it could be demonstrated that triangular hollow struts show better properties in printed templates compared to round ones, as the coating process is more homogeneous, which in turn leads to smaller defects and a more uniform induction of force. Open-celled honeycombs are shown as a CAD model in Figure **1**. Despite the significant increase in porosity of this structure compared to the dense honeycombs, initial piezoelectric measurements show d_{33} values above 200 pC,/N which exceed all expectations but must be verified with further measurements.

Additionally, BCZT powder was synthesized via an adapted sol-gel process to allow processing at lower temperatures. While typical solid-state synthesis calcination temperatures exceed 1200°C, the sol-gel process requires only 800°C, offering significant energy savings. The powder properties, density (5.78 g/cm^3), specific surface area (14.65 m^2/g), and mean particle size (d_{50} = 70.92 nm) were determined. As reference samples, replica foams with pore densities of 30 - 60 ppi (porosities between 60 - 75 vol%) were obtained from this powder. The compressive strengths ranged from 0.5 to 8 MPa, and the d_{33} values from 60 - 80 pC/N, indicating that periodic or uniform structures (honeycombs) are superior to random ones (replica) from a mechanical and piezoelectric point of view.

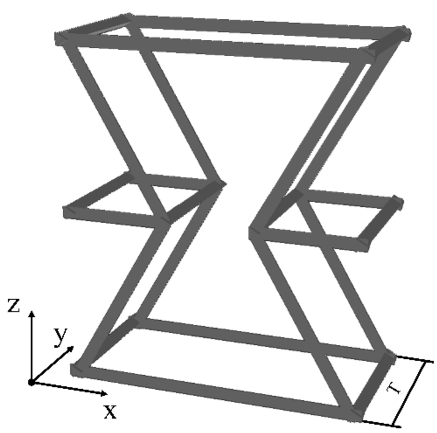


*Figure **3**: Open celled auxetic structure*

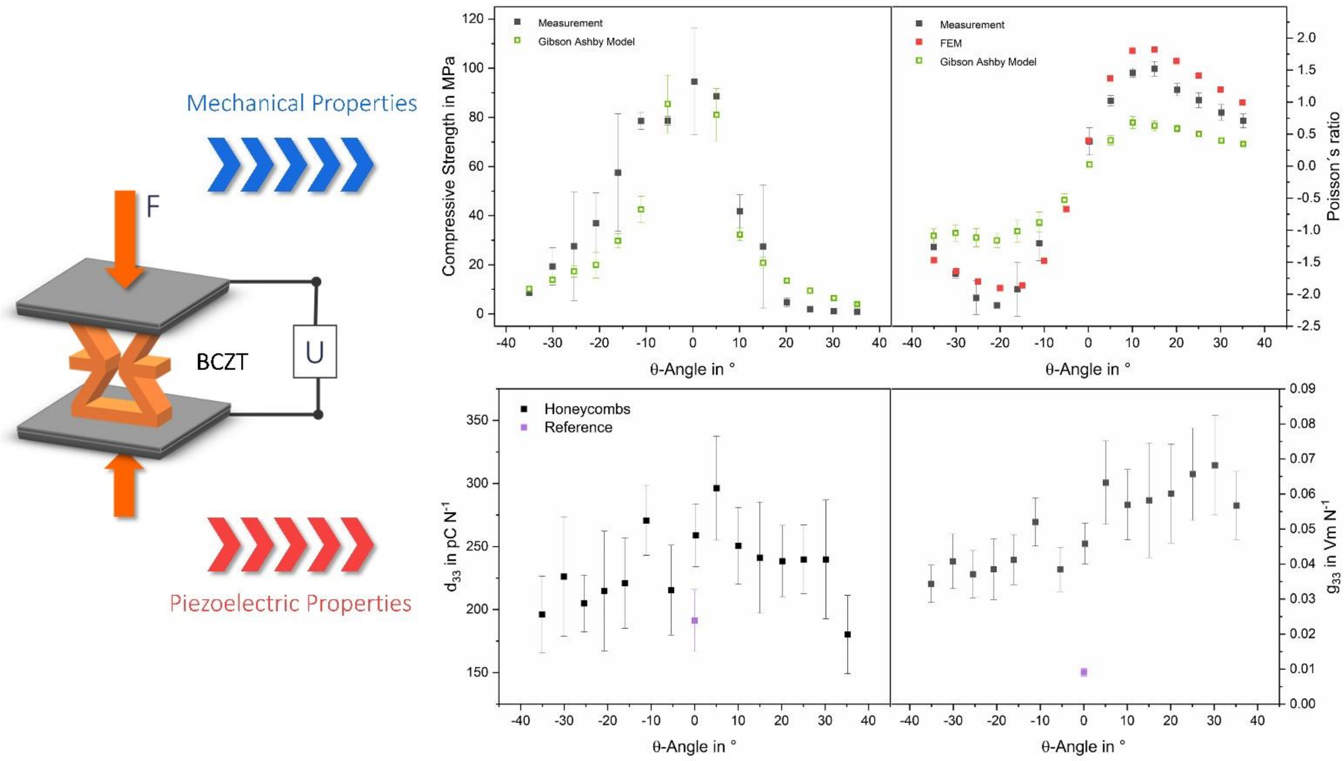


*Figure **2**: Mechanical and piezoelectric properties of BCZT honeycomb unit cells, in dependence of the structural angle.*

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

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

Objectives and status

Investigation of promising lead-free materials

Perovskites have shown great potential for future solar cell applications due their easy processability and low cost. However, one major roadblock is the presence of toxic lead in many of the best-performing perovskite cells. Thus, a search for lead-free alternatives has begun. One material family of particular interest, the Cesium-Titanium-Halides from the group of vacancy-ordered double perovskites, was investigated in this project. Pure Iodine- (Cs_2TiI_6) and Bromine-based materials (Cs_2TiBr_6) as well as mixed I/Br compounds were synthesized via mechano-chemical ball milling, characterized and the findings were published.

Microwave Photoconductivity measurements

Another important topic is the characterization procedure for newly developed photovoltaic materials. One powerful characterization technique is the measurement of microwave photoconductivity (µ-PCD), which gives insight into the charge-carrier dynamics in a candidate material. A setup to perform such measurements was already present at NITech and was successfully built up at FAU over the last two years with the help of the collaborators of Project E.

Conclusions, main achievements and outlook

Investigation of promising lead-free materials

The previous work performed on the lead-free material class $Cs_2TiBr_{6-x}I_x$ (x=0,2,4,6) was continued and augmented with scanning electron microscopy (SEM) images, XRD measurements (see Figure 4) and a crystallographic characterization. The results show that all materials exhibit a cubic crystal structure with lattice parameters of 10.70 Å (Cs_2TiBr_6), 10.88 Å ($Cs_2TiBr_4I_2$), 11.23 Å ($Cs_2TiBr_2I_4$), and 11.48 Å (Cs_2TiI_6). This project was concluded with a publication (see https://doi.org/10.1002/crat.202200150).

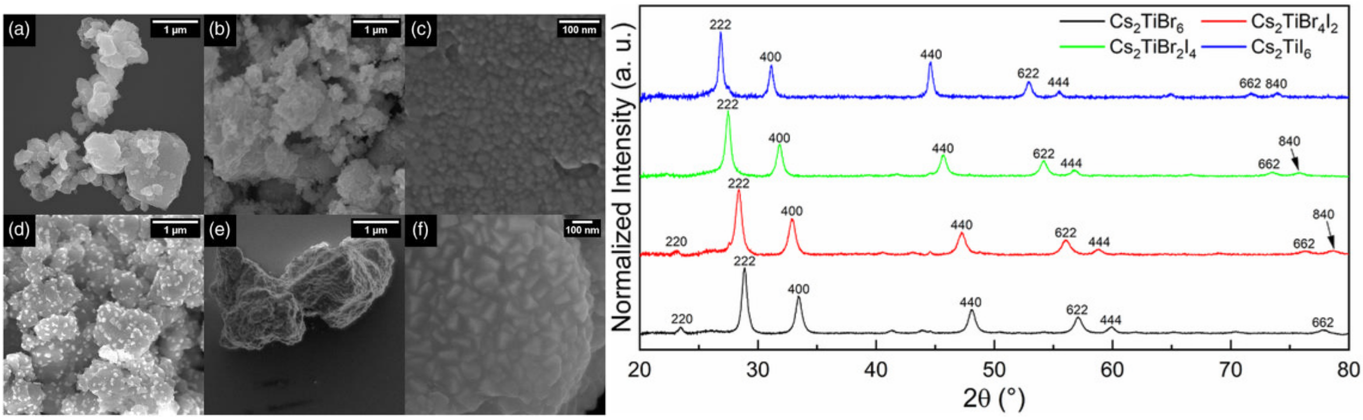


*Figure 4: **Left:** Scanning electron microscopy images of a) Cs2TiBr6 particles, b) Cs2TiBr2I4 particles, c) Cs2TiBr6 particle surface with increased magnification and visible crystallites, d) Cs2TiBr4I2 particles with bright flakes on the surfaces, originating from degradation due to exposure to ambient moisture, e) Cs2TiI6 particle, and f) Cs2TiI6 particle surface with increased magnification and visible white flakes. **Right:** X-ray diffraction patterns of cesium-titanium halides obtained by mechanochemical ball milling for 17 h at 235 RPM: Cs2TiBr6 (black), Cs2TiBr4I2 (red), Cs2TiBr2I4 (green), and Cs2TiI6 (blue). The shift of the pattern indicates a unit-cell expansion for compounds containing iodine. The most prominent peaks are labeled with their respective Miller-indices.*

Microwave Photoconductivity measurements

The newly established µ-PCD setup at FAU was first confirmed to work, then a set of reference measurements was performed at NITech during a one-month research stay to examine its performance (example measurements in Figure 5). The chosen samples were $MAPbI_3$ thinfilms on glass substrates with varying thicknesses (200-700nm), which yielded a good signal in both setups. The data was subsequently analyzed by a python program written specifically for this task. This allowed us to confirm that our setup could achieve similar results to the prototype setup at NITech. Furthermore, some insight into thickness dependent features could be gathered, although the data analysis is currently still ongoing.

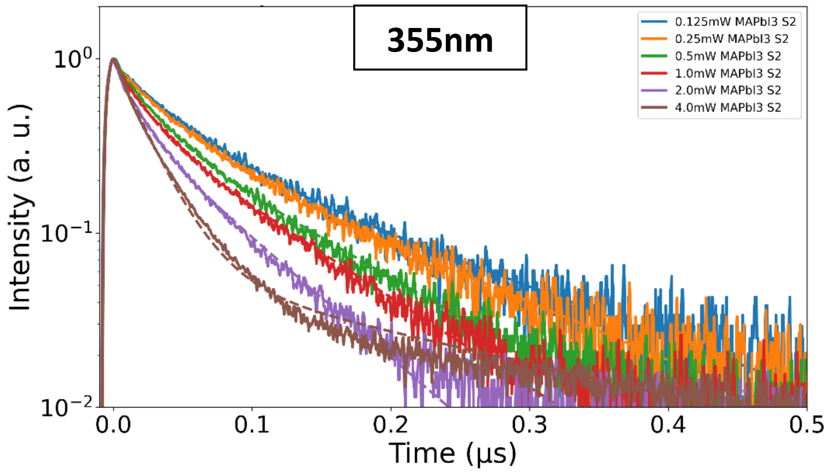


Figure 5: Microwave photoconductivity transient from 378nm thick $MAPbI_3$ thinfilm under excitation with a 355nm laser with varying intensity. Dashed lines are fits assuming a bi-exponential decay.

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

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

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. Sun, wind, and water are essential components for a sustainable energy supply. However, numerous applications do not have access to these renewable energies, such as underground sensors or remote wireless technologies, which require the use of alternative renewable sources. For example, the vibration of buildings or the movement of people can be converted from mechanical to electrical energy by piezoelectric materials and can be used to generate energy through piezoelectric energy harvesting.

A piezoelectric vibrational energy harvester (PVEH) typically consists of a substrate and a piezoelectric material. Since piezoelectric ceramics exhibit excellent piezoelectric coefficients, they are attractive for the use in PVEHs, where lead zirconate titanate (PZT) is the most commercially used material. Because of health and environmental concerns during production, usage, and disposal of lead containing materials, lead-free alternatives are required. 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 is considered for implementation in thick film energy harvesting systems. Unfortunately, the higher sintering temperature of ceramics often precludes their direct use with other substrate materials, such as metals and polymers. This problem can be overcome with aerosol deposition. 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 functional ceramic.

In this method, an aerosol is generated by a carrier gas passing through loose powder in a vibrating canister. The roughly 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 those of bulk samples. This might be due to their nanometer sized grains, internal stresses during and after AD, as well as high conductivity in as-processed films. Therefore, an annealing step is needed to activate the functional properties.

Conclusions, main achievements and outlook

Three main topics are identified:

1) Stress-induced tailoring of energy storage properties in lead-free Ba0.85Ca0.15Zr0.1Ti0.9O3 ferroelectric bulk ceramics – The corresponding paper is accepted from the Journal of Materiomics. In this study, the energy storage performance of BCZT and its tailoring by stress was investigated. It was found that the recoverable energy storage density of BCZT bulk samples can be increased by applying -160 MPa uniaxial stress by 226 % compared to the pre-stress state. At the same condition, the efficiency is increased by around 10 %. This effect is temperature stable up to 55 °C. The mechanisms behind the stress-induced increase of the energy storage performance were elucidated by polarization-stress, dielectric as well as Rayleigh measurements.

2) The influence of grain size on electromechanical properties of BCZT – Here a multiscale analysis is carried out using conventional sintered (CS) and spark plasma sintered (SPS) bulk samples as well as thick films sprayed by AD. The goal is to investigate one of the origins of the low electromechanical properties of the AD film, i.e., the nanometer sized grains. For this, AD films are compared to bulk materials. CS samples were fabricated at FAU and various SPS samples were produced at NITech varying the temperature from 1100 °C – 1400 °C, the pressure from 50 MPa – 100 MPa, and the holding time from 2 min – 10 min. The density and the dielectric and ferroelectric properties are investigated as well as their crystal structure. Importantly, their

grain size will be elucidated as well as their piezoelectric coefficient, followed by a comparison of the properties of the bulk and AD samples.

3) Investigation of annealing conditions on free-standing AD films – In this topic, AD films without substrates - so called free-standing films (FSFs) - are investigated in terms of their dielectric and ferroelectric properties. The advantage of the substrate-free approach is the possibility to investigate the annealing of AD films without the addition of microdefects due to a mismatch of the coefficient of thermal expansion with the substrate. The grain size of the FSFs increases with enhanced annealing temperature of 1400 °C up to 16 µm, which is in the same order of magnitude the grain size of bulk samples. Also, the dielectric and ferroelectric properties of FSFs increase higher annealing temperature. However, the properties of the bulk samples are not reached. This leads to the conclusion that other factors, e.g., stress, might decrease the functional properties of the FSFs as well.

Future topic in Project F: Annealing of AD films by furnace annealing and laser annealing to induce grain growth – In the furnace, the full sample is heated up. To protect the substrate nitrogen or vacuum atmosphere can be used. Also, the usage of different substrates like low expansion metals or ceramics with a similar expansion as the AD film is possible. The advantages of laser annealing are the high heating rate and the local energy input directly to the AD film, both leading to a decreased heating of the substrate and therefore less damage due to it. The collaborative project was conducted and finished with project C (NITech), C (FAU) and E. Furthermore, an energy harvester based on an annealed AD film was prepared and characterized in collaboration with Ryota Yamamoto (C). The resonance frequency was obtained and different excitation types were tested.

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

FAU: Rita Cicconi and David Dobesh
NITech: Tomokatsu Hayakawa, Koichi Hayashi, Takahito Otsuka and Kimura Koji

Objectives and status

Project G's scope includes synthesizing and characterizing parent glass compositions and evaluating the crystallization mechanisms, in order to develop glass-ceramics having functional crystals embedded in a chemical and mechanically stable, pore-free matrix. The compositional influences on parent glass structures, and crystallization mechanisms is investigated to optimize the development of glass-ceramics having applications in optics and innovative energy-related technologies (*e.g.,* second harmonic generation, down- and up-conversion, piezoelectricity, high energy-storage density). Understanding and monitoring the local glass structure evolutions will help build and design these new and efficient energy conversion materials. Additionally, the glass-ceramic method allows more variability in adjusting the chemistry to expand and tailor the material response. The crystal growth mechanisms and phases is investigated through thermal analysis and combined elemental and spectroscopic techniques.

Among the potential Pb-free polar crystals that could provide the functional properties we selected the BCZT-type perovskites. Therefore, the initial investigation was focused on developing an amorphous composition that would host high amounts of barium, zirconium and titanium. Furthermore, Europium(Eu) ions were added to the parent glasses to monitor the compositional changes. Indeed, an advanced optical characterization of the parent glasses provides a comprehensive view of the glass network and how the structure evolves through crystallization (Eu^{3+} ions as structural probe). Selection of europium was chosen to utilize the specific energy levels hypersensitive to variations in the glass structure. Additional investigations on the mechanical response of the parent glasses are necessary to create glass-ceramics with high mechanical strength and elastic properties.

Collaboration with NITech partners was of great interest due to the precise optical characterization methods. High-resolution spectra of the hypersensitive transitions utilize the Fine Line Narrowing (FLN) method in Nagoya, Japan. Additionally, the synthesis of new optical materials will expand the development of materials through the original glass-ceramic process. The crystallization of the parent glasses can also benefit from the FLN method to determine the local site occupancy within the crystal lattice.

The anticipated research goals were to investigate further the glass structure based on titanium and zirconium inclusions. The behavior of titanium is essential due to the optical energy transfer mechanisms, which may alter the optical response. Additionally, the different possible coordination environments of titanium lead to several structural roles of this cation, with large implications on the glass connectivity and also on the resulting crystallized phases. Where the crystal phases associated with piezoelectricity contain different titanium species.

Determining the glass structure morphology into crystal phases is significate for developing new energy harvesting and storing materials. Therefore, tailoring the composition of glass to crystallize specific crystal phases which have electro-optical and mechanical response applications is of great interest. The glass structure is dependent on the chemistry, which affects the potential crystal phases. The study of the local network has extended to the incorporation of Eu ions as an optical probe to determine the type of neighboring local environment.

Conclusions, main achievements and outlook

Research into the thermal evolutions of the glass matrix has been expanded and improved for understanding the formation of energy-harvesting crystal phases. Research has also evolved in determining the parent glass structure to optical and mechanical responses. The mechanical results employed unique Brillouin Spectroscopy methods at FAU in determining the transversal and longitudinal acoustic waves. The two components' sound velocity has been correlated to the elastic moduli and fracture toughness of the parent glass compositions. Optical spectroscopy has also been evaluated to couple the optical energy transfer process in determining the light management response within the compositions. The optical investigations have been studied at both FAU and NITech universities.

The combined results of the mechanical response and the crystallization mechanism have been shared at the International Congress on Glass in Berlin. The results were presented in a poster presentation and a talk during the conference. The conference provided interaction and discussion of results and research routes with the international scientific community to further develop glass-ceramic materials.

Results have been extended to quantify the crystallized phases through a new methodology that combines both in situ and ex situ methods. We have developed a surface-controlled method in the crystallization process, which monitors the type of crystal formation. The results have also been correlated to thermal properties that were evaluated in the initial phases of the research. In addition, permittivity measurements of the parent glasses exceeded the relative permittivity of commercially available glasses. Where the glass are candidates for optical displays and solar cell applications.

Research has been accomplished through a combination of vibrational and optical spectroscopy at both universities. Analysis through Raman spectroscopy provided information on the bonding environment of the glass and crystallized materials. Alterations to the composition with both zirconium and titanium were investigated on the parent glasses to correlate the precipitation of energy-harvesting crystal phases. The optical response of the glass systems has been accomplished through spectroscopic investigations at both FAU and NITech. Additionally, a new synthesis was conducted by incorporating europium ions into the glass matrix.

Europium additions to the glass displayed optical variances due to the local glass bonding types. Monitoring the evolution of the composition was done through in-person experiments at NITech in Nagoya, Japan, as part of the collaboration within Project G. The optical characterization was accomplished in Prof. Hayakawa’s laboratory, along with thermal treatments for crystallization. Synthesis of the glasses and glass-ceramics at both universities allowed for monitoring of the glass-to-crystal evolution and compositional response.

The glass structure was analyzed by investigating the optical energy transfer process to both titanium and europium doping. The parent glasses exhibited an energy transfer mechanism with titanium and zirconium variations. The doping of europium provided a luminescence center to detect the photoluminescence properties of both the glass and crystallized structures. The photoluminescent spectra offer an additional insight into the local glass structure, which relates to the precipitation of piezoelectric crystal phases from the glass matrix. Additionally, the Fine Line Narrowing technique was used at NITech, was a unique method allowing for high-resolution photoluminescence in the hypertensive transitions of the energy levels. We also investigated the local preference of Eu-ions into crystal lattices to determine the site substitution into the perovskite lattice and crystal phases. The investigation also provides broader associations in understanding the glass-to-crystal evolutions for energy-harvesting glass-ceramics materials.

H – Stress Modulated Electromechanical Coupling of Lead-Free Ferroelectrics

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

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, Raman spectroscopy, 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

The effect of varying Bi content in NBT ceramics on the temperature-dependent crystal structure has been investigated for NBT-based material with compositions $Na_{1/2}Bi_xTiO_{2.25+1.5x}$, where $x = 0.485$–0.510. These data were used to explain and compare the change in the crystal structure with the change in the mechanical and dielectric properties as a function of composition and temperature. Combined X-ray and neutron diffraction data were collected to investigate the phase composition and structure at room temperature. The element, phase distribution, and microstructure were studied by scanning electron microscopy equipped with energy-dispersive and backscattered electron diffraction detectors. An in-depth analysis of in situ high-temperature X-ray diffraction showed a good agreement with dielectric permittivity and ferroelastic stress-strain measurements as a function of temperature. The detailed results were published Journal of Applied Physics 130, 185106 (2021).

Despite the potential importance of BCZT and KNN-based for transducer applications, applied stress's influence on the macroscopic electromechanical response and the crystal structure is not well understood. Investigations of stress-and temperature-dependent properties are crucial to realize the full potential and optimize the macroscopic responses further for applications. The influence of stress on the phase boundaries of polycrystalline lead-free perovskite $(1-x)Ba(Zr_{0.2}Ti_{0.8})O_3-x(Ba_{0.7}Ca_{0.3})TiO_3$ (x= 0.4, 0.5, and 0.6) (BCZT100x) and $0.92(Na_{1/2}K_{1/2})NbO_3-(0.08-x)Bi_{1/2}Li_{1/2}TiO_3-xBaZrO_3$ (x = 0, 0.02, 0.04, 0.06, and 0.07) were characterized with small-signal relative permittivity and direct piezoelectric coefficient from −150 to 200 °C under uniaxial compressive stress up to −75 MPa for BCZT, and −150 °C to 450 °C under different constant uniaxial stress up to −200 MPa for KNN-BZ. The stress-induced suppression of the electromechanical response and shifts in the phase boundaries. For both BCZT and KNN-BZ, the interferroelectric and ferroelectric-paraelectric phase transitions were shifted to higher temperatures under the uniaxial compressive stress. Furthermore, the stress-induced shift in phase transition temperatures for BCZT was confirmed by in situ combined temperature and stress-dependent Raman spectroscopy measurements under different constant uniaxial loads (i.e., −5, −40, and −75 MPa) within the temperature range from 25 °C to 130 °C. This data was used to construct a stress-temperature phase diagram for BCZT and KNN-BZ in the vicinity of the PPB. These results are published in Journal of Material Science 57, 16581 and Journal of American Society 106, 2326.

In collaborations with researchers in Tsinghua University and our project partners at NITech, we have worked on the XFH of single crystal BCT and BCZT in order to understand the role of Ca and Zr on the lattice structure of $BaTiO_3$. Both of the resulting studies have been published in Applied Physics Letters 120, 052905 and Physica Status Solidi (b) 259, 2100609. Additionally, a new method of XFH, using the normal mode to obtain the holograph from the bulk material is still under development in SPring8, Japan. The results will be submitted to Journal of Synchrotron Radiation (see fig. 1).

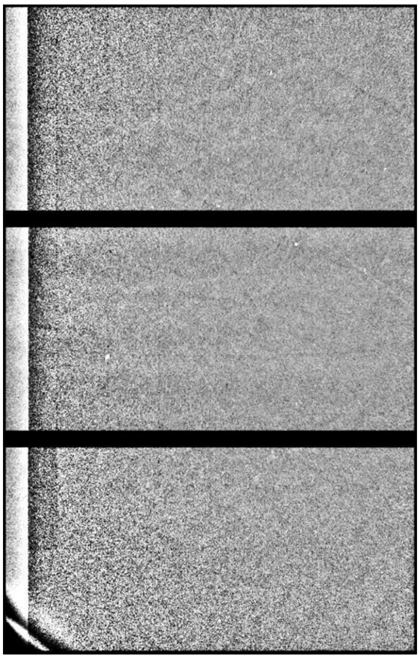


Fig. 1. Primary results of XFH normal mode of BCZT60 bulk materials.

During the research stay in NITech, the local structural changes of BCZT40-60 were obtained by pair distribution functions from synchrotron X-ray total scattering data at BL04B2 at SPring-8 (Japan). The experiment were carried out at 25–130 °C to be correlated with in situ temperature dependent Raman data for the same material at the same temperature range. Moreover, in situ high pressure Raman spectroscopy and high energy XRD were obtained for BCZT40-60 powders at NITech and Photon Factory Synchrotron (Japan), respectively. The high pressure data will be used to determine the pressure-composition phase diagram of BCZT solid solution.

I – Growth of Single Crystal Transition Metal Perovskite Chalcogenides

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

Objectives and status

The current aim of the project is to produce thin films made of Chalcogenide perovskites, specifically $BaZrS_3$ and its derivatives. Considering this, three main processing routes are being followed. These are the utilization of BaS_3 as a precursor using vacuum based processing techniques, using electrodeposition for the deposition of precursor layers and the last one being aerosol deposition for the fabrication of thin precursor films. All of those approaches follow a stacked layer approach similar to those utilized for the fabrication of $Cu(In,Ga)Se_2$ solar cells and related materials.

The successful fabrication and characterization of the precursor films is currently the main focus of the project. The synthesis of BaS_3 by annealing BaS films and powder in a sulfuric atmosphere has been achieved. The BaS initial film is prepared by electron-beam deposition. The sulfuric atmosphere is achieved by introducing elemental sulphur into the annealing chamber, which is connected to a vacuum pump. The temperature as well as the pressure of the system impact the success of this process majorly, while parameters like the amount of sulphur used and the duration of the annealing can be changed within reason without significantly changing the result. However, the morphology of the films is problematic, showing cracks and bulges most likely due to the volume expansion of the material when converting from BaS to BaS_3. It is likely, that this can be improved by optimizing the processing parameters. To do this, an improved annealing setup is currently being installed possessing the ability to control the pressure in the system precisely. Furthermore, BaS_3 as a material is not well studied, therefore the optoelectronic properties are being studied using methods like Photoluminescence and UV-VIS Absorption Spectroscopy. To study the formation of $BaZrS_3$, elemental zirconium will be sputtered upon those BaS_3 films and annealing experiments will be conducted.

Similarly, electrodeposited $ZrSe_2$ or ZrS_2 films could be used as precursors for chalcogenide Perovskites. In our lab, an electrodeposition setup was built up and continuously improved. Our initial results showed that only a small, non-stochiometric amount of Zr was incorporated into the films, indicating that elemental Se might have been deposited alongside the desired $ZrSe_2$ compound. Adjustments are currently being made in regards of the deposition solution composition, measurement settings etc. In order to produce a perovskite from these transition metal chalcogenides, another cation needs to be introduced, which would be Barium. One way to do this would be the previously mentioned BaS electron-beam deposition. Another way potentially might be intercalation, as $ZrSe_2$ and ZrS_2 are both 2-D layered materials. The respective experiments will be conducted in the upcoming months.

In Aerosol Deposition a fine powder is sprayed onto a substrate by generating an aerosol and guiding it through a nozzle into a vacuum chamber. These experiments are conducted in collaboration with Project F. In the past, it was attempted to utilize a commercially available ZrS_2 powder in this manner to manufacture a precursor film that can be combined with electron beam deposited BaS to produce $BaZrS_3$ films. Unfortunately, the properties of this powder in terms of homogeneity and size are unsuitable for this process. In the future it will be attempted to produce ZrS_2 Powder in our lab in collaboration with members of Project J which possesses suitable properties for Aerosol Deposition.

Furthermore, high temperature annealing plans around 1000°C using a stack of BaS and Zr layers will be conducted in the beginning of 2023.

Conclusions, main achievements and outlook

In the past year, advances in the production of BaS_3 films that could be utilized for the synthesis of $BaZrS_3$ thin films have been made. Currently, the goal is to better understand this formation process by improving the control over the experimental parameters like pressure and temperature and characterize the resulting films not only in terms of their composition but also optical properties. The latter will be conducted in cooperation with Professors Hayashi and Kato during Tim Freunds research stay at NITech. Particularly, Photoluminescence and Absorption measurements will be done. Raman measurements for phase identification will be conducted in collaboration with members from Project G. Additional methods for composition analysis will be X-Ray Diffraction and Energy Dispersive X-Ray Spectroscopy. To better understand the film properties, the results will be linked to computed properties. These computations will be conducted by members of Project L.

Improvements in the electrodeposition setup have been made and further studies are currently conducted.

Aerosol Deposition has been and will be conducted in collaboration with Project F.

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 three main research topics from last year were continued and are now in their final stage. In particular, the crystal growth of quasi-2D perovskites was further optimized and the synthesized crystals were characterized with respect to their optoelectronic properties. Additional experiments were then conducted for the investigation of introducing dopants into such crystals, as well as trying to replace toxic lead with less harmful bismuth.

Last year we observed self-healing properties in our x-ray detectors based on $MAPbI_3$ single crystals. To fully understand this behavior we decided to measure the photoresponsivity spectra of our crystals grown by multiple methods and correlate the results to different defect types and density. Our goal is now to do this characterization before and after x-ray induced degradation and thereby explain the existence or absence of self-healing and correlate it to a certain type of defect. This experiment will be done as soon as the new x-ray source is installed and ready at the institute.

Going further, methylammonium lead iodide single crystal solar cells were fabricated by the space-confined inverse temperature crystallization technique and finally characterized. Even though there are still some issues with the electrodes of the cells, the devices already show promising performance. Since, we had great success with this excellent growth method, it was then similarly adapted to quasi-2D and other 3D perovskites.

Conclusions and outlook

During this year V. Rehm optimized the single crystal growth of $MAPbI_3$ and multiple quasi-2D perovskites based on 3-(Aminomethylpyridine) and 4-(Aminomethylpyridine). By varying lead and ammonium precursors, cooling rate and processing of the solution, he managed to grow 1 cm sized single crystals with perfect facettes (Fig. 1). These crystals were then used for the fabrication of X-ray detectors. Since we do not have a suitable X-ray source yet, we again collaborated with Siemens Healthineers for the characterization of such devices. We found that our new crystals show decent sensitivity and a low detection limit for x-rays, while having an overall improved stability compared to the archetypical $MAPbI_3$. Our investigation of this material continued with Manganese doping experiments ,as well as trying to substitute toxic lead with less concerning bismuth. The change in properties was then monitored together with C. Kupfer from project E by doing transient photoluminescence measurements. Even with the bismuth substitution, it was still possible to grow high quality single crystals. However, due to their indirect nature they showed no photoluminescence and therefore have only limited applications in optoelectronics.

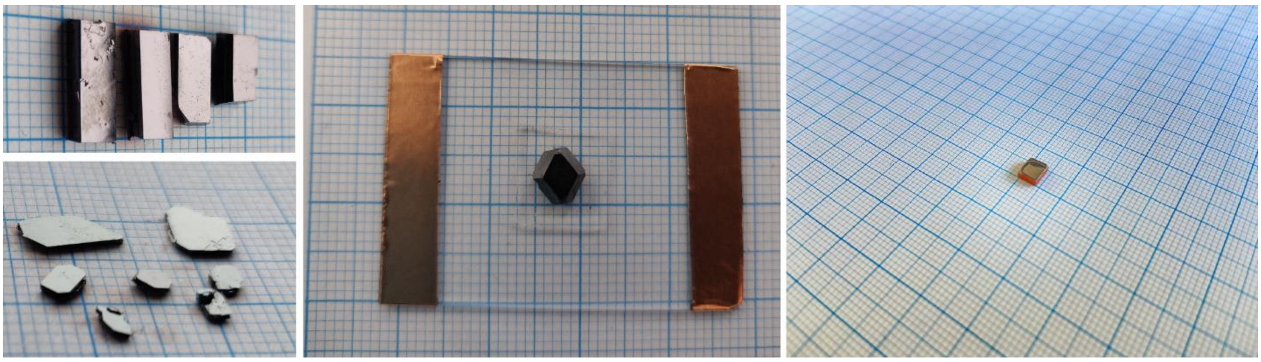


Figure 1. Some examples of single crystals and x-ray detectors

For the investigation of self-healing and its relation to intrinsic defects inside the $MAPbI_3$ single crystals, we studied their photoresponsivity spectra (Fig 2). We found out that it is possible to measure the defect density inside the crystals by doing bias dependent measurements of the responsivity. Thereby obtained values are comparable to the ones from the widely used space charge limited current method. Another important observation in the recorded spectra was the existence of a defect related peak at 850 nm. The height of this peak is strongly correlated to the concentration of triiodide ions in solution. In particular, the sample with the highest responsivity at this wavelength is the only one that showed no self-healing, which suggests a causal correlation to this type of defect. We plan to confirm our hypothesis with our new x-ray setup during this year.

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

FAU: Michael Zaiser, Frank Wendler, Dilshod Durdiev and Georgino Tshikwand
NITech: Shuji Ogata, Takahiro Tsuzuki, Ryo Kobayashi and Masayuki Uranagase

Objectives and status

The team in Project K is developing and conducting microstructure simulations to understand ferroelectric domain evolution in lead-free perovskite-based ferroelectrics under external mechanical and electrical loading, for situations relevant to materials and processing conditions within the IRTG. The scientific challenge is to map and configure a continuum model (at FAU) based on the phase-field method to molecular simulation results (at NITech), to enable the extension of simulated time and length scale as compared to atomistic simulation. In the same time specific information of defects, as local dipole moments or mechanical distortion, will enter the phase-field approach to treat problems as defect assisted domain wall motion and polarization switching.

In the actual reporting period, at FAU a settled model formulation and code base for the phase-field model was reached, and extended for 3D simulations. The numerical approach for the electro-mechanically coupled problem using a Fourier spectral method was optimized and published in a paper, where also link for the free download of the Python code is presented [1]. Also, a special focus was set on the parameter adaption from the molecular simulations. Not being as straightforward as expected, this required a tedious analysis of the phase-field energy landscape. We are able now to adapt the coefficients of the Landau-Devonshire-Ginzburg potential in connection with mechanical and electrical energy parameters to quantitatively describe domain wall energy, width, coercive field and kinetics. An ongoing effort is directed towards the quantitative agreement of the PFM with atomistic results for defect-rich perovskite ferroelectrics.

T. Tsuzuki and H. Azuma from S. Ogata's group at NITech conducted a multitude of molecular dynamics (MD) simulations for both 90° and 180° domain walls in $BaTiO_3$ with a core-shell potential approach. Analyzing the data, domain wall widths, velocities under applied electric field and polarization-field characteristics have been generated and serve as reference for the FAU continuum model. Furthermore, the Japanese partners now work on machine learning techniques to improve the predictive performance of the interaction potential.

Conclusions, main achievements and outlook

A reworking of the simulation code for the phase-field model and an extension to 3D have been carried out. We have also investigated the polarization switching process starting from a critical nucleus subjected to an applied electric field and compressive stress. A full description of the numerical scheme using the Fourier spectral method and simulations results have been published in the paper (An effective Fourier Spectral Phase-field Approach for Ferroelectric Materials, Comp. Mater. Sci.). This work includes the detailed derivation of the spectral method for ferroelectric domain evolution and polarization switching under external fields for a single crystal.

From Mai to October 2022, Takahiro Tsuzuki from NITech stayed at WW8 as a guest researcher to foster the mutual knowledge on the respective simulation approach. He conducted MD simulations for ferroelectrics with oxygen defects and provided necessary data for quantifying the properties of the material including magnitude of defect dipole moments. This ongoing work will be published in 2023, titled as "Parametrization of a phase-field model with defects from molecular dynamics data". Up to now, the coefficients of the 6^{th} order Landau polynomial have been obtained using the polarization versus field data from MD simulations, conducted by our collaborators from Japan. In addition, we also use the 180° and 90° domain wall width, domain wall velocity under applied field from MD. We have also mathematically derived how to control the 90° domain wall width. Now, we are able to control both 180° and 90° domain wall widths in the simulations.

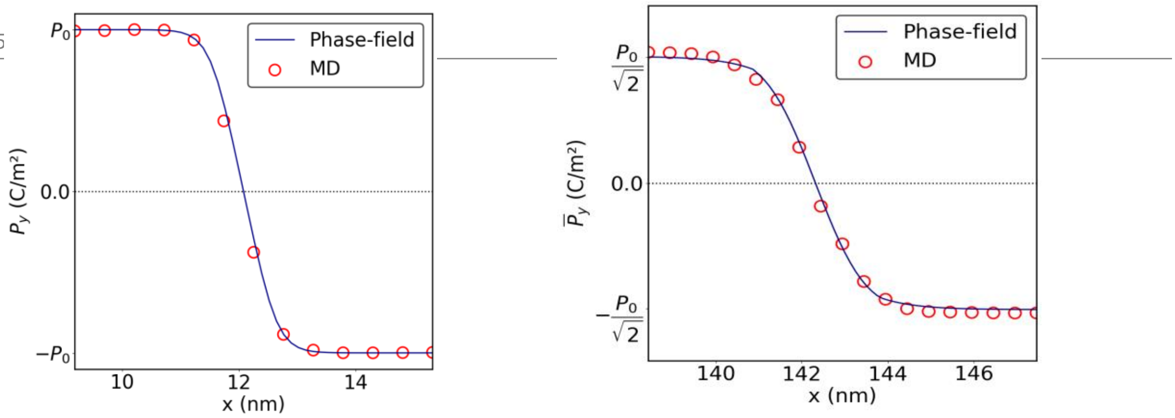


Fig. 1: *Comparison of the polarization profiles from MD and phase-field simulation, left – 180° domain wall, right – 90° domain wall.*

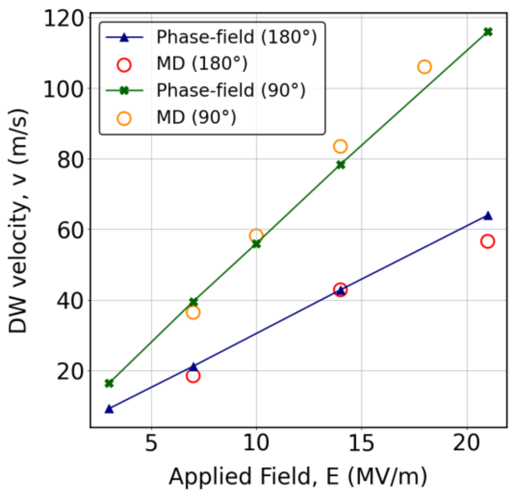


Fig. 2: *Comparison of domain wall velocities under different applied electric field from MD and phase-field. Simulations show an almost linear relationship between field and velocity.*

In the next steps, we will include point defects with localized strain and charge in our phase-field model. We assume an isotropic eigenstrain for the mechanical defect and a point charge located at the position x_0, which has been formulated as

$$\varepsilon_{ij}^{d} = \alpha\delta(x - x_0)\delta_{ij}$$
$$q^{d} = \beta\delta(x - x_0)$$

with $\delta(x - x_0)$ a Dirac delta-distribution and already included into our model. Now, simulations clarifying defects effct on domain wall kinetics and polarization switching are ongoing.

We intensified our collaborative work on photostriction with Samuele Spreafico and Bernd Meyer from Project L. The phase-field model is formulated including energy terms related to the excitation carrier density and the photo-induced stress and photo-induced electric field. These properties can be related to the polarization and strain dependency of the electric bandgap energy. S. Spreafico started DFT simulations for $BaTiO_3$ to determine these relationships. The results will enable setting up a PFM with which we study optical effects in domain wall motion and domain formation.

Former FAU MAP student Ms. Lan-Tien Hsu conducted simulation work at WW8/FAU on the relationship between electrocaloric effect and applied field orientation in $BaTiO_3$, using a coarse-grained Hamiltonian atomistic approach. She submitted her master thesis in September and is now working at RUB as PhD student in our collaborator's group (A. Grünebohm).

L – Modeling of Defect and Surface Chemistry of Perovskites

FAU: Bernd Meyer, Samuele Spreafico and Andreas Ziegler
NITech: Masaaki Haneda, Rongguang Gan and Yoshihie Nishida

Objectives and status

In this project, perovskite materials for electro-optical, electro-mechanical and catalytic applications are investigated by density-functional theory (DFT). This quantum-mechanical approach allows us to study materials on the atomic scale to derive fundamental structural and electronic properties without any *a priori* parameterization of the atomic interactions.

In 2022, Samuele Spreafico worked on three different topics. The first two are ongoing work from the previous year, the third one was started in 2022:

1) $CsPbBr_3$ quantum dots embedded in a matrix of CsBr or NaBr [1]:

Such embedded quantum dots are synthesized and characterized in the group of Wolfgang Heiss (Project J). They show very promising electro-optical properties, but their photoluminescence quantum yields depend on the matrix. The aim of the project is to obtain a better understanding of how interfaces contribute to non-radiative charge recombination in halide perovskites and how they modify the defect tolerance of these materials.

2) $Ba_xCa_{(1-x)}Ti_yZr_{(1-y)}O_3$ (BCZT) single crystals:

Ahmed Gadelmawla in project H (Webber) achieved for the first time to grow single crystals of BCZT. To complement his experimental characterization results, a computational screening was performed to determine the local atomic relaxations and their impact on the spontaneous polarization for different distributions of Ca and Zr atoms in the $BaTiO_3$ parent compound [2].

3) Photostrictive effect in bulk $BaTiO_3$:

The photostrictive effect is the mechanical response of a material to optical excitations. In a collaboration with Dilshod Durdiev from project K (Wendler) we aim at developing a multiscale approach for studying photostrictive behavior by combining atomistic quantum-mechanical calculations of photostrictive coefficients with a mesoscale phase field model [3].

Andreas Ziegler started a series of calculations to determine fundamental properties of $BaTiS_3$ (electronic structure, band gap, absorption spectrum, dielectric constants). The material is synthesized in the group of Ryan Crisp from Inorganic Chemistry and it is of special interest for solar cell application due to its stability and near-ideal band gap. Furthermore, he started to develop models of surface structures of CaO doped $BaTiO_3$, which is studied by Rongguang Gan in the group of Prof. Haneda at NITech for catalytic oxidative coupling of methane (OCM).

Conclusions, main achievements and outlook

For the $CsPbBr_3$/CsBr and $CsPbBr_3$/NaCl interfaces a screening for the thermodynamically most stable structure and composition depending on experimental synthesis conditions was performed. Subsequently, the band alignments at the interfaces were determined by calculation of projected density of states, which revealed characteristic differences for hole and electron transport depending on the interface composition. Currently, these results are refined by increasing the accuracy using computationally more expensive hybrid functionals and including spin-orbit coupling (SOC), before preparing a manuscript for submission.

A first screening was performed to find the most stable configurations of Ca and Zr atom distributions in BCZT. Then average displacements of the atoms were determined in order to get a better understanding on how the local environment of Zr and Ca atoms is modified and how this affects the spontaneous polarization P_s. The P_s values were calculated by the Berry phase approach and *via* Born effective charges to cross-check the data using two independent methods. A joint publication together with project H is currently in preparation.

In the calculations on $BaTiS_3$ two problems were encountered: First, with standard density functionals the material shows no band gap. This could be solved by applying a Hubbard-U correction to the functional. Second, it turned out that the structure proposed in the literature is not stable. After an extensive search, a new low-energy structure with a regular pattern of slightly displaced TiS_3 rows was identified. Next steps will focus on the study of the surface chemistry of $BaTiS_3$ in order to obtain insights in the observed anisotropic solution-based growth behavior of the crystallites and the properties of their ligand shells.

During his research stay at FAU in 2023, Rongguang Gan will calculate XPS signatures for the model structures of $CaO/BaTiO_3$ surfaces, which can be correlated with experimental data. This will allow us to identify important structural motifs on the surfaces and to understand better the role of surface reduction for the activation of methane and the catalytic activity of the material.

[1] Chaudhary, B., Kshetri, Y.K., Kim, H.S., Lee, S.W., & Kim, T.H. (2021). Current status on synthesis, properties and applications of $CsPbX_3$ (X = Cl, Br, I) perovskite quantum dots/nanocrystals. Nanotechnology, 32(50), 502007. https://doi.org/10.1088/1361-6528/ac2537

[2] Luo, B., Wang, X., Tian, E., Song, H., Qu, H., Cai, Z., Li, B., & Li, L. (2018). Mechanism of ferroelectric properties of $(BaCa)(ZrTi)O_3$ from first-principles calculations. Ceramics International, 44(8), 9684–9688. https://doi.org/10.1016/j.ceramint.2018.02.19

[3] Paillard, C., Prosandeev, S., & Bellaiche, L. (2017) Ab initio approach to photostriction in classical ferroelectric materials. Phys. Rev. B 96, 045205. https://doi.org/10.1103/PhysRevB.96.045205

2.1. Participation in conferences

David Dobesh

From / to	Name of the conference	Location	Title of presentation or poster, or participation only
03-08.07.2022	26th International Congress on Glass (ICG2022)	Berlin, Germany	Presentation: Titanium and Zirconium Compositional Influences on Crystallization of Glass-Ceramics for Piezoelectric Applications Poster: Inverse Glass and Crystallization Behavior of Varying Zr/Ti on Mechanical Properties

Dilshod Durdiev

From / to	Name of the conference	Location	Title of presentation/poster, or participation only
04.-08.07.2022	11th European Solid Mechanics Conference ESMC 2022,	Galway, Ireland	Presentation: A phase-field model for ferroelectrics with atomistic heterogeneity
04.-09.09.2022	DPG Meeting 2022 (German Physical Society)	Regensburg, Germany	Presentation: A phase-field model for ferroelectrics with local chemical defects

Ahmed Gadelmawla

From / to	Name of the conference	Location	Title of presentation/poster, or participation only
27.06-01.07.2022	The 2022 ISAF-PFM-ECAPD Joint Conference	Tours, France	Presentation: Stress-Temperature Phase Diagram of Lead-free (1-x)Ba(Zr0.2Ti0.8)O3-x(Ba0.7Ca0.3)TiO3)
23.-27.08.2022	The 33rd Edition of the European Crystallography Conference (ECM33)	Versailles, France	Poster: In Situ Temperature-Dependent X-ray Diffraction Study of Ferroelectric Single Crystal Ba1-xCaxTi1-yZryO3

Niharia Gogoi

From / to	Name of the conference	Location	Title of presentation/poster, or participation only
16.-17.05.2022	IEEE Sensor Interface Meeting 2022	Veldhoven, Netherlands	participation
27.06.-01.07.2022	IEEE ISAF 2022	Tours, France	Presentation: Energy harvesting from a piezo buzzer with Schottky diode and complementary MOSFET full-bridge rectifiers
30.10.-01.11.2022	IEEE Sensor 2022	Dallas, USA	Presentation: Simultaneous Step Counting and Energy Harvesting from Piezoelectric Discs Embedded in a Shoe

Andreas Hegendörfer

From / to	Name of the conference	Location	Title of presentation or poster, or participation only
06-10.03.2022	SPIE Smart Structures	Long Beach, USA	Presentation: Numerical investigation of the transient charging behavior of a piezoelectric vibration-based energy harvester for different base excitations

Patrizia Hoffmann

From / to	Name of the conference	Location	Title of presentation or poster, or participation only

10-12.10.2022	Material Science and Technology'22	Pittsburgh, USA	Presentation on: Modular Piezoceramic/Polymer composites with locally adjustable piezoelectric properties

David Köllner

From / to	Name of the conference	Location	Title of presentation or poster, or participation only
10 – 14.07.2022	ECers 2022	Krakow, Poland	Presentation: Prediction of Crack Propagation in Honeycomb Ceramics by Polarimetry and Digital Image Correlation
10-12.10.2022	Material Science and Technology'22	Pittsburgh, USA	Presentation: Prediction of Mechanical Properties of Ceramic Honeycombs by Polarimetry Measurements of Epoxy Resin Prototypes

Juliana Maier

From / to	Name of the conference	Location	Title of presentation or poster, or participation only
27.06.-01.07.2022	IEEE ISAF 2022	Tours, France	Poster: Functional Properties Relationship of Annealed Free-Standing Thick Films

Samuele Spreafico

From / to	Name of the conference	Location	Title of presentation or poster, or participation only
04.-09.09.2022	DPG Meeting 2022 (German Physical Society)	Regensburg, Germany	Poster: First-principles study of halide perovskite interface
14.-19.08.2022	CAMD Summer School – Electronic Structure Theory and Materials Design 2022	Helsinki, Denmark	participation

Simon Swantje

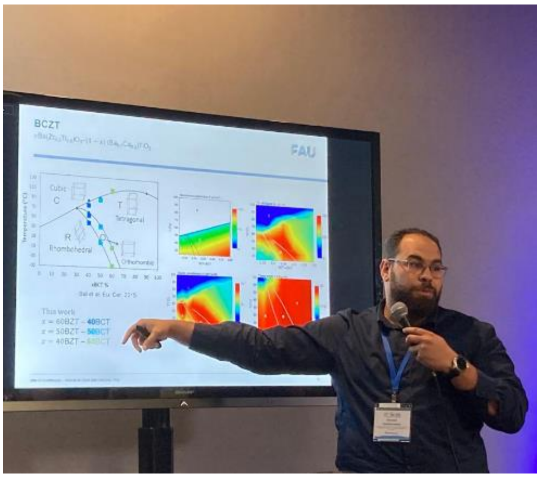
From / to	Name of the conference	Location	Title of presentation or poster, or participation only
10.-14.07.2022	Ceramics in Europe 2022 ECerS	Krakau, Poland	Presentation: Additive Manufactured Replica Foams
10-12.10.2022	Material Science and Technology'22	Pittsburgh, USA	Presentation: Periodic Cellular Ceramic Structures by Replication of Additive Manufactured Templates

Georgino Tshikwand

From / to	Name of the conference	Location	Title of presentation or poster, or participation only
28-30.06.2022	Actuator'22	Mannheim, Germany	Antagonistic SMA Film Actuators for Folding and Unfolding of Origami-Type Microstructures
03-09.07.2022	European Solid Mechanics Conference (ESMC'22)	Galway, Ireland	Self-Folding Shape Memory Microactuators for Programmable Matter

Andreas Ziegler

From / to	Name of the conference	Location	Title of presentation or poster, or participation only
14.-19.08.2022	CAMD Summer School – Electronic Structure Theory and Materials Design 2022	Helsinki, Denmark	participation


BCZT
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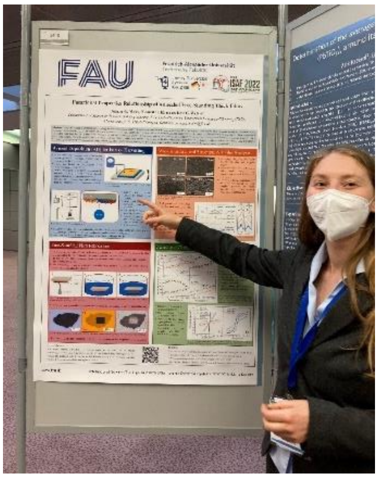
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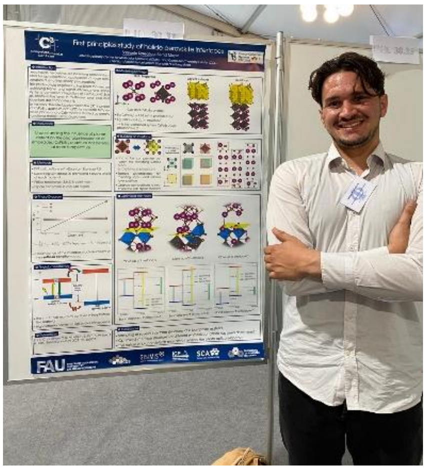
FAU


Governing equations of piezoelectricity
FAU
consider small deformations
restriction to linear piezoelectric effect, no hysteresis
mechanical
electrical
strain:
balance of lin. momentum:
Dirichlet b.c.:
Neumann b.c.:
linear constitutive law

2.2. Publications in alphabetical order

[1] **T. Otsuka, M. R. Cicconi, D. Dobesh**, B. Schroeder, **T. Hayakawa**: “93Nb NMR study of (K, Na)NbO_3-doped SiO_2-Na_2O-Al_2O_3 glasses”, Phys. Status Solidi B, (2022), DOI: 10.1002/pssb.202200016

[2] Y. Zhao, T. Heumueller, J. Zhang, J. Luo, O. Kasian, S. Langner, **C. Kupfer**, B. Liu, Y. Zhong, J. Elia, **A. Osvet**, J. Wu, C. Liu, Z. Wan, C. Jia, N. Li, **C. J. Brabec**, J. Hauch: “A bilayer conducting polymer structure for planar perovskite solar cells with over 1,400 hours operational stability at elevated temperatures”, Nat Energy 7, 144–152 (2022), DOI: 10.1038/s41560-021-00953-z

[3] **D. Köllner, J. Biggemann, S. Simon, P. Hoffmann, K.-I. Kakimoto; T. Fey**, “Additive manufactured replica foams”, Open Ceramics, 10,100258 (2022), DOI: 10.1016/j.oceram.2022.100258

[4] **D. Köllner**, B. Tolve-Granier, **S. Simon, K-I. Kakimoto, T. Fey**, “Advanced Estimation of Compressive Strength and Fracture Behavior in Ceramic Honeycombs by Polarimetry Measurements of Similar Epoxy Resin Honeycombs”; Materials, 15(7), 2361 (2022), DOI: 10.3390/ma15072361

[5] T. Samma, T. Fuchigami, S. Nakamura, **T. Fey, K.-I. Kakimoto**, “Aligned Porous Structure of (Ba,Ca)(Ti,Zr)O_3 Piezoelectric Ceramics for Enhanced Catalytic Activity”, Phys. Status Solidi B (2022), DOI: 10.1002/pssb.202100611

[6] W. Meng, J. Xu, L. Dong, J. Zhang, Z. Xie, J. Luo, B. Zhao, K. Zhang, **A. Osvet**, T. Heumüller, K. Forberich, M. Halik, N. Li, **C. J. Brabec**, “An Innovative Anode Interface Combination for Perovskite Solar Cells with Improved Efficiency, Stability, and Reproducibility”, Sol. RRL,6, 2200378 (2022), DOI: 10.1002/solr.202200378

[7] O. Stroyuk, O. Raievska, A. Barabash, **C. Kupfer, A. Osvet**, V. Dzhagan, D. R. T. Zahn, J. Hauch, **C. J. Brabec**, “$Cs_2Ag_xNa_{1x}Bi_yIn_{1y}Cl_6$ perovskites approaching photoluminescence quantum yields of 100%”, Mater. Adv., 3, 7894 (2022), DOI: 10.1039/d2ma00737a

[8] **N. Gogoi**, J. Chen, **J. Kirchner, G. Fischer**, “Dependence of Piezoelectric Discs Electrical Impedance on Mechanical Loading Condition”, Sensors, 22, 1710 (2022), DOI: 10.3390/s22051710

[9] **K. Hayashi**, M. Lederer, Y. Fukumoto, M. Goto, **Y. Yamamoto**, N. Happo, M. Harada, Y. Inamura, K. Oikawa, K. Ohoyama. **P. Wellmann**, “Determination of site occupancy of boron in 6H–SiC by multiple-wavelength neutron holography”, Appl. Phys. Lett. 120, 132101 (2022), DOI: 10.1063/5.0080895

[10] L. Wahl, **J. G. Maier**, S. Schmiedeke, T. A. Pham, **T. Fey, K. G. Webber**, N. Travitzky, **N. H. Khansur**, “Electromechanical properties of paper-derived potassium sodium niobate piezoelectric ceramics”, Journal of the American Ceramic Society 105, 6755-6764 (2022), DOI: 10.1111/jace.18655

[11] **N. Gogoi, J. Kirchner, G. Fischer**, “Energy harvesting from a piezo buzzer with Schottky diode and complementary MOSFET full-bridge rectifiers”, IEEE ISAF PFM ECAPD 2022 (Tours, France, June 27, 2022 - July 1, 2022), In: 2022 IEEE International Symposium on Applications of Ferroelectrics (ISAF) (2022), DOI:10.1109/ISAF51494.2022.9870144

[12] **M. Mehnert**, J. Faber, M. Hossain, S. A. Chester, **P. Steinmann**, “Experimental and numerical investigation of the electro-mechanical response of particle filled elastomers - Part I: Experimental investigations”, European Journal of Mechanics Volume 96, 104661 (2022), DOI: 10.1016/j.euromechsol.2022.104651

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[14] **T. Freund, M. R. Cicconi, P. Wellmann**, “Fabrication of Bariumtrisulphide Thin Films as Precursors for Chalcogenide Perovskites”, Phys. Status Solidi B, 2200094 (2022), DOI: 10.1002/pssb.202200094

[15] **G. Stankiewicz, C. Dev, P. Steinmann**, “Geometrically nonlinear design of compliant mechanisms: Topology and shape optimization with stress and curvature constraints”, Comput. Methods Appl. Mech. Engrg. 397, 11516 (2022), DOI: 10.1016/j.cma.2022.115161

[16] H. A. Afify, **M. Sytnyk, V. Rehm**, A. Barabash, O. Mashkov, **A. Osvet**, V. V. Volobuev, J. Korczak, A. Szczerbakow, T. Story, K. Götz, T. Unruh, C. Schüßlbauer, D. Thiel, T. Ullrich, D. M. Guldi, **C. J. Brabec**, **W. Heiss**, “Highly Stable Lasing from Solution-Epitaxially Grown Formamidinium-Lead-Bromide Micro-Resonators”, Adv.Optical Mater, 10 (2022), DOI: 220023710.1002/adom.202200237

[17] **A. Gadelmawla, D. Dobesh**, **U. Eckstein**, O. Grübl, M. Ehmke, **M. R. Cicconi, N. K. Khansu**r, D. de Ligny, **K. G. Webber**, “Influence of stress on the electromechanical properties and the phase transitions of lead-free (1-x)Ba(Zr0.2Ti0.8)O_3-x(Ba0.7Ca0.3)TiO_3”, Journal of Materials Science, 57 (35), 16581-16599 (2022), DOI: 10.1007/s10853-022-07685-9

[18] **N. H. Khansur, U. Eckstein**, M. Bergler, **A. Martin**, K. Wang, J-F. Li, Jing-Feng Li, **M. R. Cicconi**, K. Hatano, **K-I. Kakimoto**, D. Ligny, **K. G. Webber**, “In situ combined stress- and temperature-dependent Raman spectroscopy of Li-doped (Na,K)NbO_3”, J Am Ceram Soc., 105, 2735–2743 (2022), DOI: 10.1111/jace.18269

[19] **A. Martin, J. G. Maier**, F. Streich, M. Kamlah, **K. G. Webber**, “Investigating the importance of strain-coupling in lead-free 2-2 relaxor/ferroelectric composites with digital image correlation”, Smart Materials and Structures, 31, 075009 (2022), DOI: 10.1088/1361-665X/ac6fa0

[20] **A. Hegendörfer, P. Steinmann, J. Mergheim**, “Investigation of a nonlinear piezoelectric energy harvester with advanced electric circuits with the finite element method”, SN Appl. Science, 4, 120 (2022), DOI: 10.1007/s42452-022-05003-1

[21] S. Deumel, Y. Reg, J.E. Huerdler, L. Hussenether, O. Schmidt, A. Barabash, **W. Heiss**, S. F. Tedde, “Laser Cutting of Metal-Halide-Perovskite Wafers for X-Ray Detector Integration”, Adv. Mater. Interfaces, 9, 2200642 (2022), DOI: 10.1002/admi.202200642

[22] **Y. Yamamoto, K. Kimura, A. Gadelmawla**, K. Kawamura, H. Sugimoto, D. Liu, Q. Li, Q. Yan, **N. H. Khansur**, N. Happo, **K.-I. Kakimoto, K. G. Webber, K. Hayashi**, “Local Structural Investigation of (Ba,Ca)(Zr,Ti)O_3 and Ca(Zr,Ti)O_3 by X-Ray Fluorescence Holography”, Phys. Status Solidi B, 2100609 (2022), DOI: 10.1002/pssb.202100609

[23] **C. Kupfer**, J. Elia, **M. Kato, A. Osvet, C. J. Brabec**, “Mechanochemical Synthesis of Cesium Titanium Halide Perovskites Cs_2TiBr_6-xIx (x = 0, 2, 4, 6)”,Cryst. Res. Technol., 2200150 (2022),DOI: 10.1002/crat.202200150

[24] A. Kanak, O. Kopach, L. Kanak, I. Levchuk, M. Isaiev, **C. J. Brabec**, P. Fochuk, Y. Khalavka, “Melting and Crystallization Features of $CsPbBr_3$ Perovskite”, Cryst. Growth Des., 7, 4115–4121 (2022), DOI 10.1021/acs.cgd.1c01530

[25] **M. R. Cicconi**, R. Belli, M. Brehl, J. Lubauer, **T. Hayakawa, K. Kimura**, T. Hirota, K. Usui, S. Kohara, Y. Onodera, U. Lohbauer, **K. Hayashi**, D. de Ligny, "Nucleation mechanisms in a SiO_2-Li_2O-P_2O_5-ZrO_2 biomedical glass-ceramic: Insights on crystallization, residual glasses and Zr_4+ structural environment", Journal of the European Ceramic Society 42(4), 1762-1775 (2022), DOI: 10.1016/j.jeurceram-soc.2021.12.009

[26] **M. Mehnert**, W. Oates, **P. Steinmann**, "Numerical modeling of nonlinear photoelasticity", International Journal for Numerical Methods in Engineering (2022), DOI: 10.1002/nme.7177

[27] **D. Köllner, S. Simon**, S. Niedermeyer, I. Spath, E. Wolf, **K.-I. Kakimoto, T. Fey**, "Relation between Structure, Mechanical and Piezoelectric Properties in Cellular Ceramic Auxetic and Honeycomb Structures", Advanced Engineering Materials (2022), DOI: 10.1002/adem.202201387

[28] **C. Dev, G. Stankiewicz, P. Steinmann**, "Sequential topology and shape optimization framework to design compliant mechanisms with boundary stress constraints", Struct Multidics Optim (2022), DOI: 10.1007/s00158-022-03271-4

[29] H. A. Afify, **V. Rehm**, A. Barabash, A. These, J. Zhang, **A. Osvet**, C. Schüßlbauer, D. Thiel, T. Ullrich, M. Dierner, T. Przybilla, J. Will, E. Spiecker, D. M. Guldi, **C. J. Brabec, W. Heiss**, "Shape-Controlled Solution-Epitaxial Perovskite Micro-Crystal Lasers Rivaling Vapor Deposited Ones", Advanced Functional Materials 32(45), 2206790 (2022), DOI:10.1002/adfm.202206790

[30] **Y. Yamamoto**, K. Kawamura, H. Sugimoto, **A. Gadelmawla, K. Kimura**, N. Happo, H. Tajiri, **K. G. Webber, K. Kakimoto**, **K. Hayashi**, "Significant Displacement of Calcium and Barium Ions in Ferroelectric (Ba0.9Ca0.1)TiO_3 Revealed by X-ray Fluorescence Holography", Applied Physics Letters, 120, 052905, Feb. (2022), DOI: 10.1063/5.0076325

[31] **N. Gogoi**, Y. Zhu, **J. Kirchner, G. Fischer**, "Simultaneous Step Counting and Energy Harvesting from Piezoelectric Elements Embedded in a Shoe", IEEE Sensors Conference 2022 (Dallas, Texas, USA, October 30, 2022 –November 2, 2022), In: 2022 IEEE Sensors. DOI:10.1109/SENSORS52175.2022.9967338

[32] G. E. Eyoum, **U. Eckstein, K. Riess, A. Gadelmawla**, E. Springer, **K. G. Webber, N. H. Khansur**, "Sintering condition-dependent electromechanical behavior of the lead-free piezoelectric $Bi_{1/2}K_{1/2}TiO_3$", J Mater Sci 57, 15843–15861, August (2022), DOI: 10.1007/s10853-022-07630-w

[33] F. Eichhorn, H. Schiegerl, **D. Köllner, K.-I. Kakimoto, T. Fey**, "Stress and Deformation Behavior of 2D Composite Cellular Actuator Structures of Ceramic Building Blocks and Epoxy Resins", Phys. Status Solidi B, 2100591 (2022), DOI: 10.1002/pssb.202100591

[34] **U. Eckstein**, J. Exner, A. B. Golob, K. Ziberna, G. Drazic, H. Ursic, H. Wittkämper, C. Papp, J. Kita, R. Moos, **K. G. Webber, N. H. Khansur**, "Temperature-dependent dielectric anomalies in powder aerosol deposited ferroelectric ceramic films", Journal of Materiomics, (2022), DOI: 10.1016/j.jmat.2022.05.001

[35] **X. Shi, U. Eckstein**, S. Lang, **M. R. Cicconi, N. H. Khansur**, "Temperature-dependent ferroelastic behaviour of antiferroelectric $AgNbO_3$", Acta Materialia, 232, 117931 (2022), DOI: 10.1016/J.ACTAMAT.2022.117931

[36] **R. Yamamoto, A. Hegendörfer, J. Mergheim, K.-I. Kakimoto**, "Temperature-Dependent Vibration Energy Harvesting Performance of Polyimide/(Na,K)NbO_3 Piezoelectric Composites", Jpn. J. Appl. Phys., 61, SN1028, Aug. (2022), DOI: 10.35848/1347-4065/ac835c/pdf

[37] F. Zhuo, **U. Eckstein, N. H. Khansur**, C. Dietz, **D. Urushihara**, T. Asaka, **K.-I. Kakimoto, K.G. Webber**, X. Fang, J. Rödel, "Temperature-Induced Changes of the Electrical and Mechanical Properties of Aerosol-Deposited $BaTiO_3$ Thick Films for Energy Storage Applications", Journal of the American Ceramic Society, 105, 2735-2743, Jun. (2022), DOI: 10.1111/jace.18377

[38] Y. Ishii, S. Ishikawa, I. Yamada, K. Kondo, S. Jindo, **S. Kawasaki**, Y. Hattori, O. Mashkov, **W. Heiss**, "Ultra-fine Metal Particles Dispersed on Single-Walled Carbon Nanotubes for Energy Devices", Journal of Materials Science, Jan. (2022), DOI: 10.1007/s10853-022-06894-6

[39] **<u>M. Choi</u>, C. J. Brabec, T. Hayakawa**, "X-ray Diffraction, Micro-Raman and X-ray Photoemission Spectroscopic Investigations for Hydrothermally Obtained Hybrid Compounds of Delafossite $CuGaO_2$ and Wurtzite ZnO", Ceramics, 5, 655–672 (2022), DOI: https://doi.org/10.3390/ceramics5040048

[40] **<u>T. Tsuzuki</u>**, **S. Ogata**, **R. Kobayashi, M. Uranagase**, S. Shimoi, **<u>D. Durdiev</u>, F. Wendler**, "Vacancy-Assisted Ferroelectric Domain Growth in $BaTiO_3$ under an Applied Electric Field: A Molecular Dynamics Study", Journal of Applied Physics, 131,194101-1-10, May. (2022), DOI: 10.1063/5.0090231

2.3. Student Theses

Bachelor theses

Student	Topic	Date
Julian Guther	Charakterisierung von 2D-ZrO_2 Keramiken mit definierter Porosität	05 - 11.22
Robert Kammel	Alkali-halide single-crystal-growth for solution-epitaxy of metal-halide-perov-skites	01 - 06.22
Danica Kettner	Methodenevaluation zur Untersuchung von Subsurface Damagelayern in CdTe-Wafern nach mechanischer Bearbeitung	05 - 09.22
Aadhitya Telakula Mahesh	Alkali niobate in aluminosilicate glasses: evolution of the niobate environment depending on glass chemistry	04 - 10.22
Miklos Vermes	Auxetische piezoelektrische zellulare Strukturen	03 - 09.22

Master theses

Student	Topic	Date
Samuel Escobar	Ultra low-power wireless transmission system for self-powered piezoelectric shoe sole device	03 - 09.22
Tim Fuggerer	Fabrication, temperature treatment and characterization of ferroelectric	04 - 10.22
My An Hoang	Self-Powered Parallel SSHI Technique to Harvest Energy from Walking	11.21-06.22
Lan-Tien Hsu	A coarse-grained case study on the electrocaloric effect for non-collinear electric fields	Since 09.22
Yuanjia Zhu	Wireless data transmission from human gait	06 - 12.22

Internships

Student	Topic	Date
Yoshio Nakagawa, B.Sc., NITech	Conducted some experiments related to his Master project (Project A)	01.07.-20.09.22
Takahiro Samma, B.Sc., NITech	Investigation of the effect of cellular ceramics on piezoelectric properties for practical catalyst (Project D)	01.07.-31.10.22

2.4. Doctoral Degree

We are pleased to announce the first two successfully completed dissertation projects: Dr. Yuta Yamamoto defended his doctoral dissertation titled “Local structure analyses of perovskite materials using atomic resolution holography” on 26th March 2022. He has worked on the development of atomic resolution holography and its applications to ferroelectric perovskite materials.

Furthermore, Dr. Md Ismail Haque successfully defended his doctoral dissertation entitled “Study on Wireless Transmission from In-body to On-body and On-body to Off-body for Healthcare Purpose in an Aging Society” and got his Doctor of Engineering degree on March 26th, 2022, from Nagoya Institute of Technology.

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 2022 comprises (i) the FAU-NITech School on Energy Systems, (ii) the FAU-NITech lecture series, (iii) an international guest program (invited colloquia), accompanied by integrated soft skills training. Through feedback from doctoral researchers and PIs, this program will be continuously improved and refined.
In 2020 and 2021 we reorganized the program to hosting mostly online events to ensure that everything was available online and on-demand, and created an extensive knowledge base online. Also, in 2022 effects of the pandemic could be still felt. We kept positive aspects but went back to in-person events where possible.

Yearly School

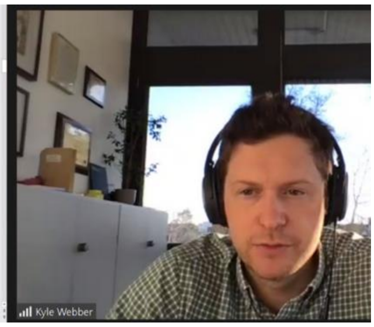
The purpose of those yearly meetings is to facilitate regular scientific exchanges between IRTG participants. Moreover, the Principal Investigator from all projects and both facilities come together to hold the bi-yearly Steering Committee Meetings.
For the second time, all of our members including PIs, Doctoral Researchers, Associated Researchers and Industrial Advisors got together online for the second Yearly School for two days. It consisted of update meetings, presentations by our doctoral researchers, two invited talks and integrated soft skills training. Before the event, all members received a small conference package – including some chocolate, a shot of ginger juice, some energy balls, mixed nuts, green tea and coffee – so everyone felt energized throughout the online meeting. Moreover, instead of pens or cups in the IRTG we had chopsticks customized with our logo which mirrors our collaboration with the Nagoya Institute of Technology (NITech) in Japan.

The Yearly School was kicked off by our IRTG director Prof. Dr. Kyle G. Webber and co-director Prof. Dr. Ken-ichi Kakimoto who welcomed everyone and presented the milestones that our IRTG could reach despite the effects of the pandemic which made live exchanges between our members in Germany and Japan impossible.

We invited two speakers to hold a presentation for our members afterwards. Prof. Webber invited Prof. Ursic from the Jozef Stefan Institute in Slovenia who investigated ferroelectric materials by atomic force microscopy, and Prof. Hayakawa from NITech invited Prof. Maeda from the Tokyo University of Science who presented his research about the brittleness of glass.

Our doctoral researchers presented previously established milestones and future research goals in their individual projects. One important aspect of this IRTG is to acknowledge doctoral researchers for their excellent scientific achievements. For that reason, already last year IRTG Young Researcher Awards have been established to recognize three doctoral researcher in the categories „Best Communication“, „Best Effort“ and „Highest Impact“. Those have been evaluated by all principal investigators and associate postdoctoral researchers. Moreover, our doctoral researchers prepared one more presentation where they showed their final results in the Collaborative Project on Integrated Coupled Energy Harvesting Systems. The doctoral researchers have been working on their projects for two years now, for which they were assigned with the following scientific question: How can one couple both phenomena – electro-optical and electromechanical – into one system? The different approaches to the questions show the interdisciplinarity of our IRTG very well: Team 1 dealt with the construction and investigation of hybrid energy harvesters. Team 2 planned designing and assembling a prototype of a cell unit, capable of harvesting solar and mechanical energy simultaneously at room temperature conditions. The aim of Team 3 was to study lead-free perovskites in regards of their photostrictive properties both experimentally and theoretically including a numerical investigation. Finally, Team 4 concentrated on energy harvesting and storing methods for electro-optical and mechanical systems. Although the evaluation results showed that Team 1 was the Winning Team, the principal investigators decided that all participants will receive a certificate for their great effort in their collaborative projects.

Since the Yearly School was held online for the second time in a row, this time we wanted to give our FAU members the chance to meet live for a team event. Therefore, FAU members met for a team challenge. The task was to create a ball path with only paper, sticks and tape. As a team, our members were able to build the ball path and on both lanes the ball reached the final point! The team success was celebrated with some Japanese food.



Young Researcher Award Winners

Takahito Otsuka | Tim Freund | Viktor Rehm

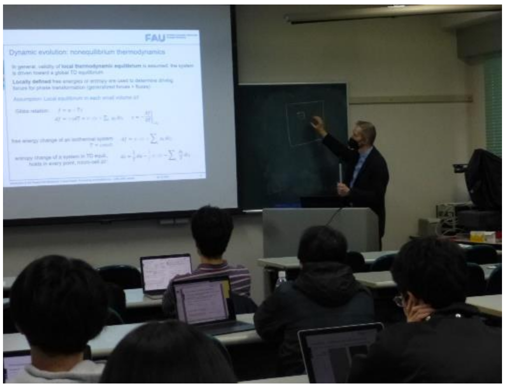
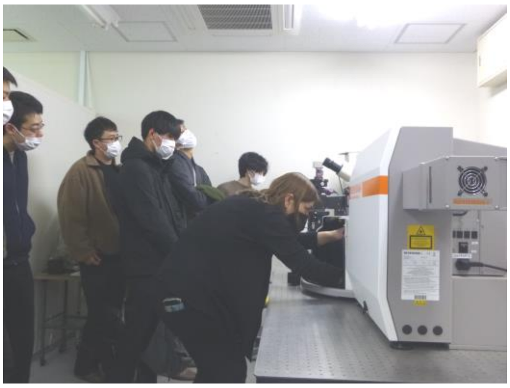
Invited Lectures

	Date	Speaker	Affiliation	Title
1	17.03.22	Jan **Schultheiß**	Norwegian University of Science and Technology, Norway	Electronic transport properties of ferroelectric domain walls – from fundamental physics to nanoelectronic applications
2	13.04.22	Yang **Bai**	University of Oulu, Finland	Photoferroelectrics for self-sustainable micro-electronics
3	05.05.22	Clive **Randall**	Materials Research Institute of Penn State University, USA	Cold Sintering of Functional Materials
4	04.07.22	Madoko **Ono**	Research Institute for Electronic Science (RIES) at Hokkaido University, Japan	Topology control of silica glass for ultralow optical scattering loss
5	21.07.22	Alexei **Gruvermann**	University of Nebraska, USA	Nanoelectronic Phenomena in Low-Dimensional Ferroelectrics
6	20.10.22	Anna **Grünebohm**	Ruhr-Universität Bochum, Germany	New concepts for cooling: Origins of the inverse electrocaloric effect
7	30.10.22	Konstantina **Lambrinou**	University of Huddersfield, UK	Accelerated Development of MAX Phase Ceramics for Advanced Nuclear Systems

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 always possible due to the on-going pandemic. However, at FAU 6 PIs and 3 PIs made an effort to make the lectures available online through recordings.
The size of the modules (5 ECTS) fit seamlessly into the academic programs of many master courses at FAU and NITech and there have been a couple of MSc students external to the IRTG who joined the lectures.

In this year, the focus of the lectures was on device development and advanced characterization techniques. The evolution of the topics from the first to the third year closely mirror the doctoral researchers' changing needs and is designed to offer information when they are ready and when they require it.

	Title	Lecturer
1	**Advanced structural characterization techniques**	
	1. Vibrational Spectroscopy of Amorphous To Nucleated To Fully Crystallized Materials	Dr. Maria Rita Cicconi
	2. Synchrotron Radiation Techniques for Materials Science	Prof. Koichi Hayashi
2	**Communication systems design**	
	1. Electronics Design for Energy Harvesting System	Prof. Georg Fischer
	2. Body Area Communications	Prof. Jianqing Wang Prof. Akimasa Hirata
3	**Advanced modeling techniques for mechano-electrical systems**	
	1. Advanced Computational Simulation of Mechano-Electrical Systems	Prof. Julia Mergheim
	2. Advanced Lecture on Motor Drives	Prof. Takashi Kosaka
4	**Crystal Growth and Material Processing – Experimental and Numerical Approaches**	
	1. Introduction to the phase-field method for crystal growth, processing and multiferroics	Dr. Frank Wendler
	2. Crystal growth of semiconductor and material processing using ultrashort laser pulses	Prof. Reina Miyagawa

Long Night of Science

On May 21st, 2022 from 6pm till midnight, the Long Night of Sciences was held in the region of Nürnberg, Fürth and Erlangen after pausing during the tough period of the pandemic. There, large scientific institutions like the Friedrich-Alexander-Universität Erlangen-Nürnberg hold lectures and demonstrations for the general public in order to present themselves and to give a general overview of their research topics. We presented our research topics such as energy harvesting, piezoelectricity as well as perovskite solar cells.
A large portion of the IoT devices cannot be powered by batteries only anymore, as they will be installed in hard to reach areas and regular battery replacement and maintenance are infeasible. A viable solution is to scavenge and harvest energy from the environment and then provide enough energy to the devices to perform their operations. This will significantly increase the device life time and eliminate the need for the battery as an energy source.

At our stand, we demonstrated an energy harvesting kit which converts mechanical vibrations into electrical energy using the piezoelectric effect. Its frequency and amplitude can be varied and so the amount of energy tuned; prepared a quiz which by visitors could prove their energy knowledge. If they checked our posters thoroughly, those who answered correctly received a matcha kit kat; we could also attract a lot of attention by our green tea station.

Tea Booth

Energy Harvester Demonstration

Workshops

Date	Presenter	Title
02.03.22	Dr. Wiebke Vogelaar (The Writing Academic)	Writing Strategies and Deep Work
28.04.22	Dr. Tobias Fey (FAU)	Preparing and Holding Lectures
27.10.22	Heidi Störr (Push your career)	Self Presentation in Job Interviews
15.-16.12.22	Dr. Friederike Schmitz (Institut für Argumentationskompetenz)	Thesis Defense Training

Writing Retreat

For Doctoral researchers it can be difficult to find time where they can work on their publications and dissertations. As work days are busy it is important to establish a routine and make time to write efficiently. This can be done for example by including deep work and Focus Sessions.

After an introduction to the concept of focus sessions by Dr. Vogelaar who is a writing coach, a 1.5 days writing retreat was held in Neuhof/Zenn. Since it was the first time for everyone to be that focused for a longer period of time, it was definitely exhausting but also productive and motivating to write in the group. This is why, we organized one day per month with focus sessions where all doctoral researchers could meet to finish some work they have procrastinated on and which they needed some extra concentration and motivation for.

3.2. Research Stays (or internships at other institutes)

David Dobesh

From / to	Institute visited	Local Supervisor	research activities performed and skills acquired
09-12.22	NITech	Prof. Hayakawa	Photoluminescence Spectroscopy and Fine Line Narrowing (FLN) Spectroscopy

Ahmed Gadelmawla

From / to	Institute visited	Local Supervisor	research activities performed and skills acquired
03.22	MAX IV Sweden	-	XFH
10-12.22	NITech	Prof. Hayashi	XFH, AXS, PDF, HP-XRD, HP-Raman, XRF

Niharika Gogoi

From / to	Institute visited	Local Supervisor	research activities performed and skills acquired
10.22	NITech	Prof. Wang	Discussion of thesis work

Andreas Hegendörfer

From / to	Institute visited	Local Supervisor	research activities performed and skills acquired
10.-11.22	NITech	Prof. Kakimoto	Simulations of energy harvesters

Christian Kupfer

From / to	Institute visited	Local Supervisor	research activities performed and skills acquired
09.-10.22	NITech	Prof. Kato	Microwave photoconductivity measurements of $MAPbI_3$ thinfilms

Juliana Maier

From / to	Institute visited	Local Supervisor	research activities performed and skills acquired
09.-11.22	NITech	Prof. Kakimoto	Fabrication of samples by spark plasma sintering (SPS), Preparing TEM and SAED investigations of free-standing films (FSFs), First energy harvesting experiment with an energy harvester based on an AD film.

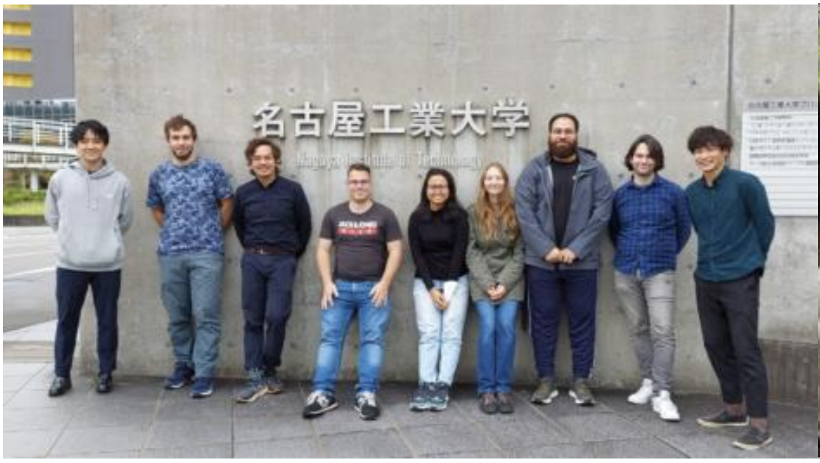
Gabriel Stankiewicz

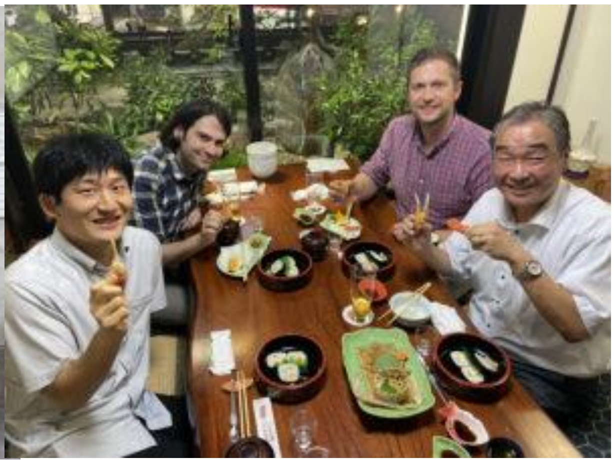
From / to	Institute visited	Local Supervisor	research activities performed and skills acquired
11.22	NITech	Prof. Kosaka	Simulation of interfaces between two orthotropic materials

Guests from NITech:

Name	From / to	activities
Ntumba Lobo	May – Oct 2022	Perovskite Crystal Growth
Asst. Prof. Daisuke Urushihara	Feb - Jul 2022	Project meeting, Electrical and mechanical property measurements for ferroelectric bulk samples
Takahiro Tsuzuki	May – Oct 2022	Analysis of BaTiO3
Takeshi Okada	Jun – Sept 2022	Finite element analysis-based simulation and optimization
Xianyi Duan	Jun – Nov 2022	Study the safety evaluation of the implantable medical devices wireless power transfer system

Ryota Yamamoto	May – Oct 2022	Finite element simulation of the piezoelectric energy harvester
Endong Zhang	Since Oct 2022	Characterization of carrier lifetime in perovskite semiconductor films formed on different substrates





3.3. Gender Equality

Next to the two cubby boxes that can be used freely at the institutes LTM or Glass and Ceramics, a family room is available for our members, as well as other scientists, employees and students from the FAU Technical Faculty. The room is equipped with a sofa, a diaper changing table, a small bed for kids, and a nice play area with a Kidsbox. While the children are playing, two tables can be used by parents as a work space. That makes it possible for mothers and fathers to spend time with their children at the university, adjourn and take care of them in cases of emergency.
The IRTG is a member of the Research Associations of Friedrich-Alexander-University Erlangen-Nürnberg for the promotion of equality (F3G). They are an association of various DFG projects at FAU and Universitätsklinikum with the aim of a better interconnection of the appropriate utilization according to principles of DFG equality funds. We financially supported F3G projects in FAU holiday childcare programme this year. Moreover, they organize workshops which our IRTG members can participate.

Workshops

	Date	Title	Organizer	Lecturer
1	30.06.2022	Implicit Bias	IGK 2495	Katrin Wladasch (factor-D)
2	18.05.2022	Making Science Visible	F^{3}G	Dr. Susanne Frölich-Steffen

Individual Coaching for female researchers

This coaching service aims to support our female scientists in their career decisions. Ms. Swantje Simon and Ms. Juliana Maier took the opportunity this year and took coaching sessions.

3.4. Monthly Meetings

It is essential to exchange scientifically and socially within the IRTG on a regular basis which is why IRTG Director Prof. Kyle Webber and Coordinator Julia Berger meet with the FAU and NITech doctoral researchers regularly, on the last Thursday or Friday of each month.

Every month we discuss organizational matters and listen to different project presentations by our researchers. In those presentations the doctoral researchers present their most recent research within a 10-minute-presentation and discuss open questions with the interested audience. Depending on the doctoral researchers interests and needs, short workshops are held. This year the topics teaching, publishing and implicit bias were addressed.

As soon as all restrictions caused by the pandemic are lifted, we will be moving to in-person meetings.

4. Appendices

4.1. Program Yearly School

Date: March 1-2, 2022	
Venue: Zoom	
Program Day 1	
08:30 – 08:30	**Opening and Welcome by Prof. Kyle G. Webber and Prof. Ken-ichi Kakimoto**
08:30 – 11:00	**Invited Talks:** Prof. Hana Ursic (Jozef Stefan Institute, Slovenia) – Investigation of ferroelectric materials by atomic force microscopy Prof. Kei Maeda (Tokyo University of Science) – How to improve the brittleness of glass? – Possibility of glass-ceramics
12:00 – 15:00	**Collaborative Project Final Presentations** Team 1: Investigation of stress-dependent material properties of Energy Harvesters Team 2: Electrooptic and Electromechanical Coupling of Photoferroic Solar Cells Team 3: In Depth Examination of Photostriction in Lead-Free Perovskites Team 4: Tailoring the conversion of a multilayered material with nano piezoelectric and phototronic effects
16:30 – 19:30	**Team Activity and Dinner**
Program Day 2	
08:00 – 12:00	**Project Presentations**
12:45 – 13:45	**Steering Committee Meeting**
13:45 – 14:00	**Awards and Final Remarks**

4.2. List of book inventory

	Author	Title	Publishing Year
1	J. Pelteret, P. Steinmann	Magneto-Active Polymers	2019
2	S. Yuji	3D Local Structure and Functionality Design of Materials	2019
3	V. Molina	Structural Models of Inorganic Crystals: from the Elements to the Compounds	2018
4	D. M. Pozar	Microwave Engineering	2011
5	R. J. D. Tilley	Perovskites: Structure-Property Relationships	2016
6	M. G. Cain	Characterisation of Ferroelectric Bulk Materials and Thin Films	2014
7	P. Schaaf	Laser Processing of Materials	2012
8	E. R. Scerri	The Periodic Table. Its Story and Its Significance	2006
9	G. Dhanaraj, K. Byrappa, V. Prasad, M. Dudley	Springer Handbook of Crystal Growth	2010
10	T. Sum, N. Mathews	Halide Perovskites: Photovoltaics, Light Emitting Devices, and Beyond	2019
11	P. Gosling	Mastering your PhD	2006
12	P. W. Atkins	Molecular Quantum Mechanics	2010
13	J. Li	Lead-Free Piezoelectric Materials	2021
14	A. King	Critical Materials (Materials Today)	2020
15	R. V. Dronskowski	Computational Chemistry of Solid State Materials	2005
16	A. Milchev	Electrocrystallization	2002
17	W. McDonough, M. Braungart	Cradle to Cradle	2002
18	A. Groß	Theoretical Surface Science	2003
19	L. Pauling, E. B. Wilson	Introduction to Quantum Mechanics with Applications to Chemistry	1985
20	D. M. Bishop	Group Theory and Chemistry	1993
21	A. Szabo	Modern Quantum Chemistry	2004
22	L.F. Chen, C. K. Ong, C.P. Neo, V. V. Varadan, V. K. Varadan	Microwave Electronics: Measurement and Materials Characterization	2015
23	M. F. Ashby	Materials and Sustainable Development	2001
24	M.E. Lines, A.M. Glass	Principles and Applications of Ferroelectrics and Related Materials	2001
25	P. Wellmann, N. Ohtani, R. Rupp	Wide bandgap Semiconductors for Power Electronics	2021
26	J. Saramäki	How to write a scientific paper	2018
27	I. Smith	Programming the Finite Element Method	2013
28	R. Tinawi	Une Présentation de la méthode des éléments finis	1983
29	D. Green	Mechanical Properties of Ceramics	2004
30	S. K. Sharma, K. Ali	Solar Cells – From Materials to Device Technology	2020
31	R. Haller	Die Entscheidung – ein Ratgeberroman über akademische Berufs-wege	2022
32	D. Tannor	Introduction to Quantum Mechanics	2018
33	B. Wang	Mechanics of Advanced Functional Materials	2013