

MAPEX Symposium 2021

Beyond solar cells: new approaches to radiation conversion

29th and 30th September 2021 online



WEDNESDAY, 29th September 2021

Session 1

9:30	Welcome address		
Tim Stauc	h, Chair of the MAPEX Symposium 2021		
Kurosch F	ezwan, MAPEX Speaker		
Marc Avila, MAPEX Human Space Exploration Initiative			
Katharina	Koschek, Poster Prize Committee		
10:00	Development of new Solar Array Concepts for Space	e Applications	
Patric See	efeldt	_	
German A	Aerospace Center, Institute of Space Systems, Breme	en, Germany	
Coffee bro	eak	<u>gather.town link</u>	
10:30 - 11:0	00		
Session 2	chair: Maciej Sznajd	er <u>zoomlink</u>	
11:00	Electrospun Polyimide Ultrafine Fibrous Membranes	with Enhanced Atomic-	
	Oxygen Resistance via Incorporation of POSS Compo	onents: Preparation and	
-	Properties		
Bohan Wu			
Beijing Ins	titute of Spacecraft Environment Engineering, China		
11:30	Poster pitches		
Odd poste	er number, see page 9		
12:00	Radiation testing of materials and prospective techn	ologies for future space	
Adrian P	Tighe		
Furopean	.Space Agency ESA / ESTEC, Noordwiik (7H). The Ne	therlands	
24.0004.1			
Lunch bre	ak	gather town link	
12:30 - 14:	00	gationcomm	
Poster ses	ssion	gather.town link	
14:00 - 15:	00		
Session 3	chair: Michael Ma	as zoomlink	
15:00	High-Z nanoparticles for enhanced energy deposition	n in tumours during	
	radiotherapy	C C	
Hans Rabi	JS		
Physikalis	ch Technische Bundesanstalt, Berlin, Germany		
15:30	Triple Halide Perovskite Absorbers for >27% Perovski	ite/Silicon Tandem Solar	
	Cells with Excellent Stability		
Michael D.	McGehee		
University of Boulder, Colorado, USA			
<u> </u>			

chair: Tim Stauch

<u>zoomlink</u>





THURSDAY, 30th September 2021

Coffee break

10:30 - 11:00

Session 5

chair: Katharina Koschek

11:00 Chemical reactions initiated by ionizing Radiation

Jan Hendrik Bredehöft

University of Bremen, Germany

Poster pitches 11:30

Even poster numbers, see page 16

12:00 Development and use of active dosimeters for ionising radiation in space

Karel Marsalek, Institute of Aerospace Medicine

German Aerospace Centre

Lunch break 12:30 - 13:30

Session 6a

chair: Patric Seefeldt

13:30 Changes in the energy consumption of private households due to the production and the use of renewable energies

Judith Maschke, artec Sustainability Research Center, University of Bremen

Poster session 14:00 - 15:00

15:00 Ternary nitrides - a disorder tunable material

Susan Schorr Helmholtz-Zentrum Berlin für Materialien und Energie, Freie Universität Berlin, Institut für geologische Wissenschaften

Prize ceremony and closing 15:30 - 16:00

Beyond solar cells: new approaches to radiation conversion

Session 4 chair: Tim Stauch 9:00 Ultrafast energy transfer through intermolecular Conical Intersections

Thomas Frauenheim

Bremen Center for Computational Materials Science, University of Bremen, Germany

Donor/acceptor interfaces in organic and hybrid materials for photovoltaics: Insight from first-principles calculations

Caterina Cocchi

9:30

Carl von Ossietzky Universität Oldenburg, Humboldt-Universität zu Berlin, Germany

10:00 Overview of radiation damage mechanisms in materials

Kai Nordlund

University Helsinki, Finland

<u>zoo</u>mlink

gather.town link

gather.town link

gather.town link

zoomlink

zoomlink



zoomlink

zoomlink

Virtual participation

Talks via zoom

All talks will be broadcasted via the video conferencing platform zoom. You can join the meeting via the zoom app, your browser or your telephone.

For participation please use the following link or ID and code:

https://uni-bremen.zoom.us/j/96357007916?pwd=TjdacmNscmRUeWJBTzcyTHpiKzZVUT09

- meeting ID: 963 5700 7916
- code: 570938

Detailed information and alternatives for participation are also summarized on a special website, which can be accessed via the following link:

www.uni-bremen.de/mapex/symposium-2021/programme/virtual-participation

All participants except the speaker will be muted by default. Recordings and Screenshots are not allowed.

For questions to the speakers during the discussion just raise your hand in zoom.

For technical questions please use the private chat function addressing the support (Jan or Guilherme).



Breaks and poster sessions via gather.town

For the breaks and poster sessions we have set up a virtual workshop environment on the platform gather.town. Here you will use your personal avatar to walk around the poster room and venue. Every poster will have its 'private area' for individual discussions, similar to a conventional poster session.

We encourage you to use the breaks on gather.town for networking with other colleagues.

https://gather.town/invite?token=-2nus4BA6nDMv6XAlRBYlzOILsikhxZ5

Welcome to the MAPEX Symposium 2021





Live event for networking

We have chosen a special place for a live networking event Wednesday afternoon in Bremen, starting about 30 minutes after the last talk at 4:30 pm:

DAV Kletterzentrum Bremen Robert-Hooke-Str. 19 (next to the turnaround loop of tram no 6)



Participation is free, we will offer some snacks and drinks. A small selection of dishes can be ordered at your own expense.

Due to the special situation (Corona) special rules apply:

- additional registration via email is necessary (there is an upper limit of participants)
- the 3G rules apply: This means that you have to be vaccinated, recovered, or tested ("geimpft, genesen oder getestet") in order to participate. We will check your status upon entering the building.



Wednesday, 29th September 2021

Session 1, 9:30 - 10:30

<u>zoomlink</u>

Chair: Tim Stauch

9:30 Welcome address

Tim Stauch, Chair of the MAPEX Symposium 2021 Kurosch Rezwan, MAPEX Speaker Marc Avila, MAPEX Human Space Exploration Initiative Katharina Koschek, Poster Prize Committee

10:00 Development of new Solar Array Concepts for Space Applications

Patric Seefeldt

German Aerospace Center, Institute of Space Systems

Bremen, Germany

Solar arrays are the main power source in space. Conventionally they are composed of stiff backing structures and brittle PV cells. While the power demands of space missions are increasing, e.g. for electric propulsion, the increase of efficiency of the solar cells itself is limited. New developments make use of flexible and semi-flexible solar array designs in order to achieve higher power/mass and power/volume ratios. An example is a twodimensional deployment of solar arrays in order to increase the deployed area as instigated in DLR's GoSolAr project. Such deployment strategies can be combined either with conventional photovoltaics, also using thinned wafer technology, or with thin-film technologies that are truly flexible. Development of such technology involves also deployment testing and testing of materials under the specific radiation environment that is present in space. In this talk I would like to give an overview about the development aspects, showing how we try to go beyond conventional array designs but still using photovoltaic solar cells.



Patric Seefeldt is a 39 years old mechanical engineer with a diploma (RWTH Aachen 2010) and a PhD (University of Bremen 2018). As deputy head of the Mechanics and Thermal Systems Department (since 2016) and head of the Material Aging Group (since 2019) at DLRs' Institute of Space Systems, he is pursuing research in the field of innovative applications of new materials for space technologies.

Coffee break, 10:30 – 11:00 gather.town link



Session 2, 11:00 - 12:30

zoomlink Chair: Maciej Sznajder

11:00 Electrospun Polyimide Ultrafine Fibrous Membranes with Enhanced Atomic-Oxygen Resistance via Incorporation of POSS Components: Preparation and Properties

Bohan Wu

Beijing Institute of Spacecraft Environment Engineering

Polyimide (PI) represents a class of important materials in various space applications due to their high thermal resistance, good dielectric and mechanical properties, which make PIs good candidates for thermal control materials, electrical insulating coatings, solar cell substrates, and other protecting components on spacecraft. However, when the standard PIs are exposed to the severe space environment, they are subject to degradation of the thermal optical property through oxidation and etching by atomic oxygen (AO) in low Earth orbit (LEO). AO is created by the dissociation of molecular oxygen caused by solar ultraviolet radiation at wavelengths below 243 nm. Such property degradation has been a serious impediment for application of PIs for spacecraft. Therefore, the protection of PIs from long-term AO erosion has become one of the most important issues to be addressed in the design and manufacturing of spacecraft components operating in LEO. The PI films and composites have been most widely studied for the protection purpose from AO erosion. However, few works on the AO erosion and protection research on the PI fibers or fabrics have been reported up to now although PI fibers have increasingly attracted attention in space application. In this talk, I would like to present the most recent work in our lab on the AO resistance of PI nanofibrous membranes (NFMs) incorporated with POSS.



Dr. Wu Bohan has been working as a senior engineer at Beijing Institute of Spacecraft Environment Engineering since 2014. Her expertise is ground-based space environmental simulation, space material evaluation, and development of AO protection materials. She worked as a Postdoctoral Research Associate at the University of Basel, Switzerland and at Montana State University, USA. She got her PhD in Physical Chemistry at the University of

Nottingham, UK. She has experience in the general field of physical chemistry with specialization in cluster science, molecular dynamics, high-resolution spectroscopy, and materials science.



Session 2: poster pitches, 11:30 - 12:00

<u>zoomlink</u>

The eff	fect of photonic crystals on the efficiency enhancement of	
	Nada Amadi	
PUI	Neud Allidui Department of Rasic Sciences	
	Garmsar Branch Islamic Azad University Garmsar Iran	
Develo	unment of In-Situ Measuring Techniques and Synergetic Radiation of	
Materia	als for Space Application.	
P03	Erik Klein	
	Institute for Space Systems, University of Bremen, Germany	
Activit	y and Mechanism Mapping of Photocatalytic NO $_2$ Conversion on the	
Anatas	ie TiO ₂ (101) Surface	
P05	Pu Guo	
	Bremen Center for Computational Materials Science	
01.11	University of Bremen, Germany	
Stackii	ng engineering: A boosting strategy for 2D photocatalysts	
P07	Yan Liang Bromon Contor for Computational Matorials Science	
	University of Bromon, Gormany	
Artifici	al Solar Wind for Space Material Developments	
	Patric Seefeldt	
105	German Aerospace Center (DLR) – Institute of Space Systems	
	Bremen. Germany	
Ultrafast Photoinduced Electron Transfer in Endohedral Fullerene Mg@C60		
P11	Mohamed El-Amine Madjet	
	Bremen Center for Computational Materials Science	
	University of Bremen, Germany	
Localiz	ed Orbital Excitation Drives Bond Formation in Plasmonic Catalysis	
P13	long Mou	
	Snenznen JL Computational Science and	
Fana D	Applied Research Institute, Guangaong, China	
Fano Resonance and incoherent interlayer Excitons in Molecular van der Waals Heterostructures		
P15	Carlos Medrano	
	Bremen Center for Computational Materials Science	
	University of Bremen, Germany	
Design of a ceramic/polymer cell for harvesting proton radiation in extra-		
terrest		
PI/	I di ija Lili ik Advanced Ceramice, University of Premen, Cermany	
	Auvunceu Cerunnics, University Or Breinen, Germuny	



12:00 Radiation testing of materials and prospective technologies for future space missions

Adrian P. Tighe

European Space Agency, ESA / ESTEC, Noordwijk (ZH), The Netherlands

In this talk I will give an overview of some of the challenges related to the radiation testing of materials for space applications, describing some of the test facilities and techniques, showing results of investigations our group in ESTEC has performed as well as discussing prospective materials technologies which could be utilized for radiation energy conversion for future space missions.



Dr. Adrian Tighe is a senior materials engineer working for the European Space Agency, where he leads the environmental testing group within the Materials Physics and Chemistry Section, utilizing an array of advanced state-of-the-art vacuum facilities to simulate the effects of the space environment on materials.

Lunch break, 12:30 – 14:00 gather.town link

Poster session, 14:00 - 15:00

gather.town link

We kindly ask all authors of posters with odd numbers to be present at their posters for discussion.

Poster prizes

The Royal Society of Chemistry with its new journal "Energy Advances" is sponsoring two poster prizes, 100 \in each.

One prize will be awarded for each poster session / day.

During the last session of the day, all participants will vote on the winner of the day via zoom. Both winners will be honoured on Thursday during the award ceremony.



Session 3, 15:00 - 16:00

<u>zoomlink</u> Chair: Michael Maas

15:00 High-Z nanoparticles for enhanced energy deposition in tumours during radiotherapy

Hans Rabus

Physikalisch Technische Bundesanstalt, Berlin, Germany

Radiotherapy is a trade-off between tumour control and unwanted side effects in healthy tissue. Both radiation effects depend on the absorbed dose, i.e. energy imparted per mass. Due to proliferation, cancer cells are susceptible to radiation damage. This opens the so-called therapeutic window, i.e. a dose range where treatment efficacy exceeds the risk of side effects, whose width is fixed by biological factors. High-Z nanoparticles offer the prospective to selectively enhance energy deposition in tumours while sparing healthy tissue.



Hans Rabus graduated in surface science at Freie Universität Berlin and then worked for 27 years in radiation metrology at PTB, Germany's National Metrology Institute, were he was leading for 11 years the department "Radiation Effects" in the Ionizing Radiation division.



Triple Halide Perovskite Absorbers for >27% Perovskite/Silicon 15:30 **Tandem Solar Cells with Excellent Stability**

Michael D. McGehee

University of Boulder, Colorado, USA

Wide bandgap metal halide perovskites are promising candidates to pair with low bandgap silicon, copper indium gallium diselenide, or perovskite photovoltaics for highly efficient next-generation tandems due to excellent optoelectronic properties, low-cost manufacturability, and bandgap tunability. Here, we alloy chlorine into the perovskite lattice to create a triple halide wide bandgap perovskite absorber, a phase space that has thus far been overlooked. We show that chlorine is incorporated into the lattice in molar amounts up to 15%. The addition of chlorine doubles the charge carrier mobilities and lifetimes of the material. We show that a 1.67 eV triple halide perovskite does not experience photoinduced halide phase segregation under intensities up to 100 suns. Finally, we incorporate triple halide perovskite into solar cells, obtaining single junction devices with open-circuit voltages >1.2 V and >20% efficiency, and monolithic perovskite/silicon tandem solar cells with voltages approaching 1.9 V and >27% efficiency. Solar cells with the triple halide perovskite absorber retain 95% of their initial efficiency under maximum power point tracking at 60°C under white light illumination for 1000 hours.



Mike McGehee is a Professor in the Chemical and Biological Engineering Department at the University of Colorado Boulder. He is the Associate Director of the Materials Science and Engineering Program and has a joint appointment at the National Renewable Energy Lab. He was a professor in the Materials Science and Engineering Department at Stanford University for 18 years and a Senior Fellow of the Precourt Institute for Energy. His current research interests are

developing new materials for smart windows and solar cells. He has previously done research on polymer lasers, light-emitting diodes and transistors as well as transparent electrodes made from carbon nanotubes and silver nanowires. His group makes materials and devices, performs a wide variety of characterization techniques, models devices and assesses long-term stability. He received his undergraduate degree in physics from Princeton University and his PhD degree in Materials Science from the University of California at Santa Barbara.



Thursday, 30th September 2021

Session 4, 9:00 - 10:30

zoomlink

Chair: Tim Stauch

9:00 Ultrafast energy transfer through intermolecular Conical Intersections

Thomas Frauenheim Bremen Center for Computational Materials Science University of Bremen, Germany

Conical intersections (Colns) of multidimensional potential energy surfaces are ubiquitous in nature and control pathways and yields of many photoinitiated intramolecular processes. Such topologies can be potentially involved in the energy transport in aggregated molecules or polymers but are yet to be uncovered. By using ultrafast two-dimensional electronic spectros- copy (2DES), we reveal the existence of intermolecular Colns in molecular aggregates relevant for photovoltaics. Non-adiabatic dynamics simulations identify an intermolecular Coln as the source of these unusual ultrafast dynamics.



Since 2006 Chair Professor for Computational Material Science, Bremen Center for Computational Material Science, University of Bremen https://www.bccms.uni-bremen.de/cms/

2019: 1000-Talent Award of China for Foreign Senior Scientist and since 2020 Chair Professor at Computational Science Research Center (CSRC) Beijing, https://www.csrc.ac.cn/en/people/faculty/181.html



9:30 Donor/acceptor interfaces in organic and hybrid materials for photovoltaics: Insight from first-principles calculations

Caterina Cocchi

Carl von Ossietzky Universität Oldenburg, Germany Humboldt-Universität zu Berlin, Germany

Donor/acceptor interfaces are ubiquitous building blocks of organic and hybrid materials for optoelectronic and photovoltaic applications. In-depth understanding of their electronic and optical characteristics is therefore essential to gain full control on their structure and properties. First-principles methods such as (time-dependent) density-functional theory [1] and manybody perturbation theory [2] offer an ideal trade-off between accuracy and numerical complexity to complement experiments in the study of these systems. In this talk, I will analyze electronic and optical response of doped organic semiconductors [3-5] in relation with experiments [6-8]. I will also discuss the earliest stage of formation of coherently driven optical transitions in a prototypical hybrid inorganic/organic interface, focusing on the critical role of electron-vibrational coupling and on its influence on the chargetransfer mechanisms [9].

References:

J. Krumland, A. M. Valencia, S. Pittalis, C. A. Rozzi, and C. Cocchi, J. Chem. Phys. 153, 054106 (2020).
C. Cocchi and C. Draxl, Phys. Rev. B 92, 205126 (2015)

[3] A. M. Valencia and C. Cocchi, J. Phys. Chem. C 123, 9617 (2019)

[4] A. M. Valencia, M. Guerrini, and C. Cocchi, Phys. Chem. Chem. Phys. 22, 3527 (2020).

[5] R. Schier, A. M. Valencia, and C. Cocchi, J. Phys. Chem. C 124, 14363 (2020).

[6] A. E. Mansour, D. Lungwitz, T. Schultz, M. Arvind, A. M. Valencia, C. Cocchi, A. Opitz, D. Neher, and N. Koch, J. Chem. Mater. C 8, 2870 (2020).

[7] M. Arvind, C. E. Tait, M. Guerrini, J. Krumland, A. M. Valencia, C. Cocchi, A. E. Mansour, N. Koch, S. Barlow, S. R. Marder, J. Behrends, and D. Neher, J. Phys. Chem. B 124, 7694 (2020).

[8] C. P. Theurer, A. M. Valencia, J. Hausch, C. Zeiser, V. Sivanesan, C. Cocchi, P. Tegeder, and K. Broch, J. Phys. Chem. C 125, 6313 (2021).

[9] M. Jacobs, J. Krumland, A. M. Valencia, H. Wang, M. Rossi, and C. Cocchi, Adv. Phys. X 5, 1749883 (2020).



Caterina Cocchi received her PhD in physics from the University of Modena and Reggio Emilia, Italy, in 2012. She moved to Germany in 2013, first as post-doctoral scientist and then, from April 2017, as Junior Professor for "Theory of excitations in low dimensional systems" at the Physics Department of the Humboldt-Universität zu Berlin. Since April 2020 she is full professor of "Theoretical solid state physics" at the University of Oldenburg.

10:00 Overview of radiation damage mechanisms in materials

Kai Nordlund

University Helsinki, Finland

Harvesting energy from any particles with kinetic energies exceeding the energy of chemical bonds, i.e. energies above a few eV, raises the possibility that the particles introduce permanent damage in the materials used for the conversion. The mechanisms by which energetic particles have been examined systematically since the 1950's, and are very well understood in some cases, and poorly in others. In this talk, I briefly review the basic physics understanding, stemming both from experiments and simulations, of radiation effects induced in hard condensed matter by ions and photons. I also consider as a specific case study what kind of damage is expected to be produced by solar wind protons in semiconductor materials.



Kai Nordlund is professor of computational materials physics and dean of the Faculty of Science at the University of Helsinki. He received his PhD in physics in 1995 at the University of Helsinki, and after postdoc positions at the University of Illinois and Academy of Finland was appointed full professor at his alma mater in 2003. He is leading a 20-person research group doing quantum mechanical, classical and mesoscale atomistic simulations of radiation and other non-equilibrium effects in all classes of materials.

Coffee break, 10:30 – 11:00 gather.town link



Session 5, 11:00 - 12:30

zoomlink Chair: Katharina Koschek

11:00 Chemical reactions initiated by ionizing Radiation

Jan Hendrik Bredehöft

University of Bremen. Germany

Conventional wisdom has it that the chemical changes caused by ionizing radiation are due to the formation of radicals and their subsequent (re-) combination. This is especially true in the field of Astrochemistry, where ionizing radiation is the primary driver for chemical conversion. There are, however, problems with this theory. I will, in this talk, briefly explain the ways that ionizing radiation can interact with matter, before giving an overview of the (sometimes surprisingly specific) kinds of chemical reactions that follow.



Jan Hendrik Bredehöft is a physical chemist with an interest in the prebiotic evolution of biomolecules and the eventual emergence of life. In 2017 he received his Habilitation from the University of Bremen, where he heads the Astrochemistry group, studying the interaction of (secondary) electrons with condensed matter.



Simulation of the interaction of polymer/ceramic composite materials with		
ionizing space radiation		
P02	Chieh-Min Hsieh	
	Institute for Physical and Theoretical Chemistry	
	University of Bremen, Germany	
Role of electron-induced chemistry in a resist for extreme ultraviolet		
	Detra Swiderek	
F 04	Institute for Applied and Physical Chemistry	
	University of Bremen, Germany	
Ultrafa	ast optically induced ferromagnetic state in 2D antiferromagnetic-	
ferromagnetic van der Waals Heterostructures		
P06	Shuo Li	
	Department of Physical and Macromolecular Chemistry Prague,	
	Czech Republic	
Energy transfer and charge recombination in an artificial molecular		
photo	catalytic system	
P08	Fulu Zheng	
	Bremen Center for Computational Materials Science	
Electri	University of Bremen, Germany	
P10		
1 10	Bremen Center for Computational Materials Science	
	University of Bremen, Germany	
Theory	y meets experiments for laser-induced processes on TiO ₂ anatase 101	
surfac	e: O_2 activation role in CO photo-oxidation.	
P12	Adrian Dominguez-Castro	
	Bremen Center for Computational Materials Science	
	University of Bremen, Germany	
Photoinduced Ultrafast Spin Transfer Dynamics in 2D Magnets and van der		
Waals	Heterostructures	
P14	Junjie He	
	Bremen Center for Computational Materials Science	
Ontes	University of Bremen, Germany	
Br. I) semiconductor studied by First Principle calculations"		
P16	Mumtaz Manzoor	
0	Riphah International University, Lahore	
	1	



12:00 Development and use of active dosimeters for ionising radiation in space

Karel Marsalek

Institute of Aerospace Medicine, German Aerospace Centre

Cosmic radiation is one of the limiting factors for long-duration space missions. For the assessment of radiation risk for humans DLR has been developing among others active radiation detectors for usage (i) onboard ISS, (ii) satellites, (iii) Moon orbit and surface, (iv) and for exploration missions. DLR works on models of the radiation field and cross-benchmarks the models and the radiation detectors. In the talk, we present development steps of a dosimeter and show dosimetry data from several space missions.



Karel is since 2002 research fellow at German Aerospace Centre, he leads the electronics development of active instruments for dosimetry of cosmic radiation in space. PhD in biomedical engineering in 2000. Current activities: Artemis I (Orion MPCV) payload development (MARE), Astrobotic Moon Lander Payload, MATROSHKA III ISS dosimetry suite.

Lunch break, 12:30 - 13:30 aather.town link



Session 6a: 13:30 - 14:00

<u>zoomlink</u> Chair: Patric Seefeldt

13:30 Changes in the energy consumption of private households due to the production and the use of renewable energies

Judith Maschke artec Sustainability Research Center University of Bremen, Germany

In order to achieve the goals of the German energy transition changes in the energy consumption of private households are also required. In this context, efficiency, consistency and sufficiency strategies should be considered. The talk presents the results of a study that dealt with the question of what effects the own production and/or use of renewable energies has on the energy consumption of private households. In addition to changes in everyday actions, the focus is also on rebound effects.



I'm a research assistant at the artec Sustainability Research Center of the University Bremen with a background in politics and sustainability. My focus is on sustainable (energy)consumption and rebound-effects.

Poster session, 14:00 - 15:00

gather.town link

We kindly ask all authors of posters with even numbers to be present at their posters for discussion.

Poster prizes

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Session 6b: 15:00 - 15:30

<u>zoomlink</u>

Chair: Patric Seefeldt

15:00 Ternary nitrides - a disorder tunable material

Susan Schorr

Helmholtz-Zentrum Berlin für Materialien und Energie, Abteilung Struktur und Dynamik von Energiematerialien Freie Universität Berlin, Institut für geologische Wissenschaften

Ternary nitrides $ZnMIVN_2$ (MIV= Ge,Sn) are being considered as promising candidates for photovoltaic absorber materials, containing uniquely elements of low toxicity and low resource criticality [1]. It has been postulated based on DFT calculations that these compounds possess a mechanism for bandgap tuning through cation disorder [2].

We are using diffraction techniques to investigate the crystal structure and structural disorder of $Zn_{1+x}Ge_{1-x}(N_{1-x}O_x)_2$ (x<0.35) which allows us to distinguish between intrinsic and compositional cation disorder. Finally the relationship between cation disorder and the bandgap energy is discussed.

[1] Narang, et al., Adv. Mater. 26 (2014) 1235-1241.

[2] Skachkov, et al., Phys. Rev. B. 94 (2016) 205201.



Susan Schorr has a diploma in crystallography and a PhD in physics. She is the head of the Department Structure and Dynamics of Energy Materials at the Helmholtz-Zentrum Berlin and teaches at the Freie Universität Berlin.

15:30 closing and poster prize ceremony <u>zoomlink</u>

Poster prizes

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One prize will be awarded for each poster session / day.



Collection of abstracts of poster contributions

P01

The effect of photonic crystals on the efficiency enhancement of semitransparent organic solar cells

Neda Ahmadi,^a

Department of Basic Sciences, Garmsar Branch, Islamic Azad University, Garmsar, Iran

We have designed the semitransparent solar cells and used the two-dimensional (2D) photonic crystals (PC) in the active layer and investigated the optical parameters of this structure. We have utilized Finite-difference time-domain (FDTD) method for our simulation and show that the effect of 2D photonic crystals on optical parameters. The sunlight ranging wavelength is from 300-1100 nm. We used Al with thickness 500nm as a cathode and Zinc oxide (ZnO) as a cathode interface layer (CIL) with a thickness 70nm. Moreover, we used Indium tine oxide (ITO) with thickness 178nm as anode and Poly (3,4-ethylenedioxy thiophene) : poly (styrene sulfonate) (PEDOT:PSS) was used as an anode interface layer.

The polymer donor poly[2,60-4,8-di(5-ethylhexylthienyl)benzo[1,2-b;3,3-b 2[dithiophene]-alt-[3-fluoro-2[(2-ethylhexyl)carbonyl]thieno[3,4-b[thiophenediyl] (PTB7- Th)with the visible absorbing fullerene acceptor [6,6]-phenyl-C71-butyric acid methyl ester(PC71BM), PTB7-Th:BC71BM is an active layer where fitted from [1]. The absorbed power spectra of PTB7-Th: PC71BM are shown in Fig. (1) for devices without and with PC. We can see PTB7-Th : PC71BM has stronger visible absorption and the photonic crystals modify the absorption spectra. The spectral range from 313 to 345 nm, from 445 to 539 nm, and from 816-1100nm absorbed power for structure with PC is more than structure without PC.

Literature: [1] S. Zhang, Y. Qin, J. Zhu, J. Hou, **Adv.Mater.** 30, e1800868.





P02 Simulation of the interaction of polymer/ceramic composite materials with ionizing space radiation

Chieh-Min Hsieh^a

^aInstitute for Physical and Theoretical Chemistry, University of Bremen

This project aims at simulating polymer/ceramic composite materials interacting with ionizing radiation by employing density functional theory (DFT) calculations. The results of simulation will provide rational design ideas for a novel material that generates electric power by utilizing ionizing radiation in space. As a starting point, hybrid solar cells, which consist of an organic electron acceptor and an inorganic electron donor, are studied by simulation techniques. Since the HOMO-LUMO energy gap and the band offset of the electron donor/acceptor are crucial parameters for evaluating the efficiency of energy generation of hybrid solar cells, a benchmark of DFT calculations of the HOMO-LUMO energy gap is conducted. Algorithms such as quasiparticle GW [1] and GLLB-sc [2] implemented in the GPAW code [3], which have been reported to predict the HOMO-LUMO energy gap in excellent agreement with experimental results, are used to calculate the HOMO-LUMO energy gap of organic semiconductors such as perylenetetracarboxylic dianhydride (PTCDA) and poly-3-hexylthiophene (P3HT). At a later stage of this project, modelling direct interaction of protons with materials and identifying the degradation mechanism will be the main focal points and will possibly point out a promising technique that slows down the degradation of materials caused by ionizing radiation.

Keywords: DFT, GW, GLLB-sc, HOMO-LUMO energy gap, hybrid solar cell, ionizing radiation

Literature: [1] F. Hüser et al., **Phys. Rev. B** 87, 235132. [2] M. Kuisma et al., **Phys. Rev. B**, 82, 115106.

[3] J. J. Mortensen et al., Phys. Rev. B, 71, 035109.



P03 Development of In-Situ Measuring Techniques and Synergetic Radiation of Materials for Space Application.

Erik M. Klein^{a,b}, Patric Seefeldt^b, Maciej Sznajder^b

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Abstract for the introducing poster on the planned and partially carried out activities during the third PhD project of the APF Seed 2 Project "Materials on Demand".

Humans reach further and further into interplanetary space. This makes the development of novel technologies and materials necessary to further support life outside of Earth's atmosphere. At the Centre for Materials and Processes (MAPEX) Bremen, new materials to shield, sense and possibly harvest space radiation are developed, simulated and tested by three doctoral projects respectively. The latter, the here introduced project which includes the testing, will be conducted at and builds up on the already existing Complex Irradiation Facility (CIF) at DLR's Institute of Space Systems (IRS).

The work aims for the validation of the developed materials through testing under simulated space radiation environment since the actual environment is rarely directly accessible during a technical development phase. For this purpose, it is intended to simultaneously use different corpuscular and electromagnetic radiation sources of the CIF.

Thus, to realize the stated goals, initially, an understanding of the space environment ruling certain reference scenarios is prerequisite. This is conducted by applying adequate models that characterize the different environments (e.g. Earth orbits and interplanetary space). Then, by considering the capability of the facility and analysis of the materials to some extent, test parameters will be defined and irradiation conducted. Evaluation of the materials will also require new means of measuring material properties and monitoring of the different radiation sources (e.g. beam profile of corpuscular radiation). Furthermore, by analysis and simulation of the facility, the resemblance of the artificial space environment with its natural counterpart shall be improved. Conclusions will be drawn, by again consulting the reference mission scenarios and comparing them to the irradiation results.

P04 Role of electron-induced chemistry in a resist for extreme ultraviolet lithography (EUVL)

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The chemistry driven by low-energy electrons plays a decisive role in processing of materials with ionizing radiation. A highly topical example are state-of-the-art nanofabrication processes that were also the subject of recent European concerted research networks [1,2]. In focused electron beam induced deposition (FEBID), low-energy secondary electrons (LESEs) released upon impact of a keV electron beam on a surface dissociate adsorbed metal organic precursor molecules to generate a solid deposit. Extreme ultraviolet lithography (EUVL) applies 92 eV photon irradiation through a mask to locally transform a resist layer and thus imprint patterns on surfaces. EUV absorption releases photoelectrons (PEs) that again create LESEs. To unravel the role of these electrons, we have studied a novel EUVL Zn oxocluster resist by monitoring volatile species that desorb from the resist during electron irradiation as well as by infrared spectroscopy of pristine and irradiated samples [3]. The results show in fact that low-energy electrons together make a substantial contribution to the resist chemistry that leads to the desired solubility switch upon EUV absorption.



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Phys. Chem. Chem. Phys. 23, 16646-16657 (2021). 2021 PCCP HOT Article

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 722149



P05 Activity and Mechanism Mapping of Photocatalytic NO $_2$ Conversion on the Anatase TiO $_2(101)$ Surface

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NOx emission heavily affects our environment and human health. Photocatalytic denitrification (deNOx) attracted much attention because it is low-cost and nonpolluting, but undesired nitrite and nitrate were produced in reality, instead of harmless N_2 . Unveiling the active sites and the photocatalytic mechanism is very important to improve the process. Herein, we have employed a combinational scenario to investigate the reaction mechanism of NO₂ and H_2O on anatase TiO₂(101). On the one hand, a polaron-corrected GGA functional (GGA + Lany-Zunger) was applied to improve the description of electronic states in photoassisted processes. On the other hand, a reaction phase diagram (RPD) was established to understand the (guasi) activity trend over both perfect and defective surfaces. It was found that a perfect surface is more active via the Eley-Rideal mechanism without NO₂ adsorption, while the activity on defective surfaces is limited by the sluggish recombinative desorption. A photogenerated hole can weaken the OH* adsorption energies and circumvents the scaling relation of the dark reaction, eventually enhancing the deNOx activity significantly. The insights gained from our work indicate that tuning the reactivity by illumination-induced localized charge and diverse reaction pathways are two methods for improving adsorption, dissociation, and desorption processes to go beyond the conventional activity volcano plot limit of dark conditions.



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P06 Ultrafast optically induced ferromagnetic state in 2D antiferromagneticferromagnetic van der Waals Heterostructures

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To understand the time scales of magnetization in two-dimensional (2D) magnetic materials is a fundamental physical point and a significant interest for technical applications. For ever- increasing speed of data storage in spintronic devices, faster methods for manipulating the magnetization in 2D magnetic materials to keep pace with computation rates of modern processors. Therefore, understanding these basic properties within the limit of ultrafast timescales is of fundamental interest. Light is the fastest means to manipulate the spin injection and transfer of 2D magnetic van der Waals (vdW) heterostructures. Theoretical research on optically induced spin dynamics in 2D materials may help to foster the development of 2D spintronics devices. The quantum properties of 2D materials can be effectively adjusted by magnetic vdW interfacial engineering. With inspired by the recent discovery of 2D ferromagnetic (FM) transitional metal dichalcogenides and antiferromagnetic (AFM) MXenes, we applied the real-time density functional theory to study optically induced interlayer spin transfer dynamics in 2D antimagnetic-ferromagnetic (AFM-FM) vdW heterostructures, for example Cr2CCl2-MnS2 interfaces (Figure 1). We observed that laser pulses induce significant large spin injection from TMDs to MXenes and phase transfer from AFM to FM states in MXenes within a few femtoseconds. Our results provide the microscopic understanding for optically control interlayer spin dynamics in 2D magnetic heterostructures and open a new way to manipulate magnetic orders in AFM spintronics.



Figure 1 optically induced FM state in 2D AFM-FM Cr2CCl2-MnS2 Heterostructures

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P07 Stacking engineering: A boosting strategy for 2D photocatalysts

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Two-dimensional (2D) photocatalytic material is a vital project for modern solar energy conversion and storage.[1] Despite a vast family of potential 2D photocatalysts is demonstrated, their commercial applications are severely limited because of fast photogenerated electron-hole recombination.[2] Based on non-adiabatic molecular dynamics within the framework of density functional theory,[3] we propose a general paradigm to boost the separation of photoexcited charge carriers in 2D photocatalysts by stacking engineering. Taking the emerging water splitting photocatalyst MoSi₂N₄ as an example, we show that specific interlayer stacking-induced electric polarization plays a significant role in altering the electronic properties and thus the suppressed recombination rate of photoexcited carriers. Moreover, the catalytic performance can be further controlled by vertical strain. These generalized findings not only highlight the importance of stacking-induced electric polarization, but also offer new prospects for the design and application of 2D photocatalysts.

Literature:

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P08 Energy transfer and charge recombination in an artificial molecular photocatalytic system

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Recently molecular photoncatalytic systems (MPSs) have drawn increasing attention for their potential applications in artificial photosynthesis. A supramolecular membrane based photosynthesis system is designed and synthesized by combining vesicle membranes and porphyrin MPSs. The MPSs exhibit high photocatalytic stability and long photocatalytic lifetime in aqueous solution. By performing non-adiabatic excited state molecular dynamics for porphyrin monomer and dimer systems, we explore the photoinduced energy transfer and charge recombination in these systems. It is found that, compared with the monomer, the porphyrin dimer exhibits faster energy relaxation and slower charge recombination. Therefore, the J-aggregated porphyrin channels generated inside vesicle membrane not only prompt the intermolecular exciton transfer, but also contribute to the long photocatalytic lifetime. We believe the present work has provided a practical way to break through the lifetime bottleneck of MPSs.

P09

Artificial Solar Wind for Space Material Developments

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German Aerospace Center (DLR) – Institute of Space Systems, Bremen, Germany Investigating materials under space environment conditions requires the artificial recreation of both corpuscular and electromagnetic radiation under ultra-high vacuum conditions. DLR's Complex Irradiation Facility combines a proton and an electron accelerator as well as electromagnetic radiation sources with broad wavelength range from ultraviolet radiation to infrared radiation in one facility. It is used to investigate the aging of materials in simulated space environment.

Literature:

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Electric Field Tunable Ultrafast Charge Dynamics in vdW Heterostructures

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^oShenzhen JL Computational Science and Applied Research Institute, Shenzhen, China Van der Waals (vdW) heterostructure are emerging platforms for investigating the concept and design of functional heterostructures for applications in the areas of electronics, photonics, renewable energies, etc. [1] The newly developed graphene/transition metal dichalcogenides (TMDCs) heterostructure with superior light-absorption properties of TMDCs [2] and high electrical conductivity of graphene [3] has been taken as potential materials for novel optoelectronic devices. [4] This drives many experimental and theoretical studies focusing on the ultrafast charge transfer process at graphene/TMDCs heterointerfaces. [5]. Here, we study the photo-induced charge transfer in graphene/WS₂ heterostructure by time-dependent density functional theory molecular dynamics. Our results show that holes transfer from graphene to WS₂ two times faster than electrons, and the occurrence of interlayer charge transfer is found correlated with vibrational modes of graphene and WS2. It is further demonstrated that the carrier dynamics can be efficiently modulated by external electric fields. Detailed analysis confirms that the carrier transfer rate at heterointerface is governed by the coupling between donor and acceptor states, which is the result of the competition between interlayer and intralayer relaxation processes. Our study provides insights into the understanding of ultrafast interlayer charge transfer processes in heterostructures and broadens their future applications in photovoltaic devices.



Figure Illustration of electric field tunable interlayer charge transfer in graphene/WS₂.

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Ultrafast Photoinduced Electron Transfer in Endohedral Fullerene Mg@C60

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Photoinduced charge transfer (CT) is a key process in organic photovoltaics whose donor-acceptor complexes are predominantly based on fullerene materials. This is because a fullerene molecule can be chemically tuned by choosing its endohedral core [1] or exohedral ligands including polymers [2,3] to control light absorption efficiency and carrier transport. Upon absorbing a photon, the energy converts to an exciton that either dissociates into free carriers or recombines depending on the electron-hole separation and excitonic binding energy. Of course, the dissociation is preferred for photovoltaics [4]. Thus, the decay and transfer of a "hot"electron from one location of the molecular material to another is a fundamental sub-process of this mechanism. Therefore, gaining insights into the CT dynamics by addressing a simpler prototype system is very important.

In this work, we investigated electron relaxation and transfer in Mg@C60 after a localized photoexcitation of Mg atom. The electron dynamics processes are investigated using nonadiabatic molecular-dynamics (NAMD) simulations in combination with time-dependent density functional theory (DFT) **[5]**.

Literature:

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Theory meets experiments for laser-induced processes on TiO_2 anatase 101 surface: O_2 activation role in CO photo-oxidation.

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TiO₂ is one of the most promising candidates for excellent applications in photocatalysis because of its low costs, and structural properties, chemical stability, and high photocatalytic activity.[1–3] Studies of photo-induced reactions on TiO₂ are crucial to the development of efficient technology responsible for air and water purification and environmental remediation.[4–6] The photochemical oxidation of carbon monoxide (CO) to carbon dioxide (CO₂) catalyzed by TiO₂ is important for air purification.[2] Theoretical calculations are an effective strategy to complement and understand the experimental results in atomistic details. Our study predicts that the presence of intragap unoccupied O₂ levels leads to the formation of a charge-transfer complex. This allows the reaction to be initiated following laser illumination at a photon energy of 1.6 eV (770 nm), taking place via a proposed mechanism involving the direct transfer of electrons from TiO₂ to physisorbed O₂. These findings highlight that it is also possible to trigger the photoreaction on TiO₂ with visible light rather than the conventional electron/hole formation.

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Localized Orbital Excitation Drives Bond Formation in Plasmonic Catalysis

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Localized surface plasmons generated on metallic nanostructures offer an alternative method for accelerating chemical transformations. However, the overall efficiency is limited because of the challenge to control the energy/charge transfer at the metal/molecule interfaces. Here, using the reduction of nitrophenol as a prototype reaction, we report density functional theory calculations showing a reduced activation barrier on an Au(111) surface for nitrophenol activation under electronic excitation; in parallel, we observed higher reaction rates on Au nanoparticles under visible-light irradiation. Furthermore, a heterostructure was constructed to represent Au@carbondoped BN (Au@CBN), which presented a significantly reduced activation barrier for nitrophenol activation. We concluded that the beneficial effects result from targeted molecular orbitals being decoupled electronically from the extended s states in Au using the thin film of CBN. This work thus provides mechanistic insights on the plasmonic bond formation and a valuable strategy for optimizing catalytic efficiency.





P14 Photoinduced Ultrafast Spin Transfer Dynamics in 2D Magnets and van der Waals Heterostructures

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Two-dimensional (2D) magnets and van der Walls (vdW) heterostructures open unprecedented opportunities for discovering emergent phenomena and implementing device structures in all-2D spintronics. Although light is the fastest means to manipulate the magnetism, interfacial spin injection and magnetic proximity related quantum properties of 2D magnetic materials and vdW heterostructures, its potential remains mostly untapped. Using real-time density functional theory (rt-TDDFT) with non-collinear spin, we show demonstrate that laser pulses can directly induce ultrafast spin selective charge transfer between magnetic sublattices in a few femtoseconds and further generate dramatic changes in the magnetic structure of ferrimagnetic (FiM) MXenes, including a transition from FiM to transient ferromagnetism (FM).[1] The microscopic mechanism behind this ultrafast switching of spin is governed by the optically induced intersite spin transfer (OISTR) effect, which theoretically enables the ultrafast optical manipulation of the magnetic state in 2D magnets. On the other hand, using rt-TDDFT simulations, we studied photoinduced interlayer spin transfer dynamics in 2D nonmagnetic-ferromagnetic (NM-FM) vdW heterostructures, including graphene-Fe3GeTe2, silicene- Fe3GeTe2, germanene- Fe3GeTe2, antimonene- Fe3GeTe2 and h-BN- Fe3GeTe2 interfaces. We observed that laser pulses induce significant large spin injection from Fe3GeTe2 to nonmagnetic (NM) layers within a few femtoseconds. [2] In addition, we identified an interfacial atom-mediated spin transfer pathway in heterostructures in which the photoexcited spin of Fe first transfers to intralavered Te atoms and then hops to interlayered NM layers. Interlayer hopping is approximately two times slower than intralayer spin transfer. Our results provide the microscopic understanding for optically control intralayer and interlayer spin dynamics in 2D magnets and vdW heterostructures.

Photoinduced Interlayer Spin Transfer



Figure 1: Photoinduced interlayer spin transfer in 2D Fe3GeTe2 and nonmagnetic materials.

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Beyond solar cells: new approaches to radiation conversion



Fano Resonance and Incoherent Interlayer Excitons in Molecular van der Waals Heterostructures

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Complex van der Waals heterostructures from layered molecular stacks are promising optoelectronic materials offering means to efficient, modular charge separation and collection layers. The effect of stacking in the electrodynamics of such hybrid organic-inorganic two-dimensional materials remains largely unexplored, whereby molecular scale engineering could lead to advanced optical phenomena. For instance, tunable Fano engineering could make possible on-demand transparent conducting layers or photoactive elements, and passive cooling. We employ an adapted Gersten-Nitzan model and real time time-dependent density functional tight-binding to study the optoelectronics of self-assembled monolayers on graphene nanoribbons. We find Fano resonances that cause electromagnetic induced opacity and transparency, and reveal an additional incoherent process leading to interlayer exciton formation with a characteristic charge transfer rate. These results showcase hybrid van der Waals heterostructures as paradigmatic 2D optoelectronic stacks, featuring tunable Fano optics and unconventional charge transfer channels.

Literature:

Carlos R. Lien-Medrano, et al., Fano Resonance and Incoherent interlayer excitons in molecular van der Waals heterostructures, 2021, https://arxiv.org/abs/2108.07364v2.



Optoelectronics applications of agryrodite Li2PS5X (X = Cl, Br, I) semiconductor studied by First Principle calculations

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We discussed and calculated the argyrodite compound with the full-potential linearized augmented plane wave (FLAPW) method[1]. To solve the Exchange Correlations in agryrodite we used the WIEN2k code by applying the Perdew burke Ernzurhof-generalized gradient approximation (PBE-GGA) potential. We calculated the structural, electronic Band structure and density of states as well as optical (real, imaginary dielectric function, reflectivity, E-loss, absorption, refractive index and excitintion coefficient) properties. It observed that it is good candidate for optoelectronics devices.

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P17 Design of a ceramic/polymer cell for harvesting proton radiation in extra-terrestrial environments

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The overall project aims to develop new types of composite materials for space travel, which will protect against ionising space radiation, measure radiation exposure and convert its inherent energy into electricity. In order to realise this goal we focus on material development, simulation and interaction with space radiation, particularly proton radiation originating from the sun.

Here, we demonstrate first steps to develop a thin cell that interacts with proton radiation to generate electricity. The investigated principle is based on a semiconductor junction and the specific interaction of ceramic nanoparticles with ionising radiation. Here, two different mechanisms apply: as a result of collisions with mobile protons, electrons can either be ejected from the shell of the atoms in the nanoparticles as low energy secondary electrons (LEE) or they can be excited into a higher energy level in analogy to a the working principle of a photovoltaic cell. The proposed cell structure and its concept including the energy levels that will be developed for this purpose can be seen in Figure 1.



Figure 1: From left to right: cell structure and cell concept

The selected nanoparticles are cerium oxide (CeO_2) and tantalum pentoxide (Ta_2O_5) , as these are already used in proton cancer therapy for their ability to enhance LEE generation. The electron transport layer can consist of organic or inorganic materials. For the latter, TiO₂ and ZnO are suitable candidates. When selecting organic materials, care must be taken to ensure that the polymers are conducting and thus are based on a conjugated Π -system. Here, fullerene, polyacetylene and perylene diimide-based polymer systems will be investigated. Silver and gold are used as electrode materials. For the actual cell design, simulations were used for the selection of possible materials and required layer thicknesses. Various methods for creating thin layers have been evaluated in preliminary experiments and will be followed by testing of the cells in a simulated space radiation environment.



Organizing committee

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Tim Stauch is a tenure-track professor for Theoretical Chemistry at the University of Bremen. He obtained his PhD in the group of Andreas Dreuw in Heidelberg and worked as a postdoc with Martin Head-Gordon at UC Berkeley. His research focuses on computational materials science and deformed molecules.

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Hanna Lührs is the science manager of the MAPEX Center for Materials and Processes since 2015 and teaching in the masters programme process-oriented materials research. She did her PhD at the University of Bremen in Crystallography and has a background in geosciences and materials mineralogy.

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Katharina Koschek is currently head of Department Mechanical Polymeric Materials and Engineering, Fraunhofer Institute for Manufacturing Technology and Advanced Materials IFAM in Bremen where she works since 2012. After studying chemistry in Leibzig she did her PhD at Freie Universität Berlin the and the Leibniz-Forschungsinstitut für Molekulare Pharmakologie. Katharina's group is working in Organic and Polymer Chemistry developing advanced fiber reinforced plastics. She is also teaching at University of Bremen's Faculty of Production Engineering focusing on engineering relevant polymer concepts.



Michael Maas

Advanced Ceramics University of Bremen, Germany



Michael Maas is a senior scientist at the Advanced Ceramics group at the University of Bremen. He studied chemistry at TU Dortmund and completed his PhD in Physical Chemistry in 2008, also at TU Dortmund. He then spent two years as a postdoc at Stanford University after which he joined the University of Bremen where he habilitated in 2018. Research Areas: Colloidal assembly of multifunctional nanostructures; Organic/inorganic Hybrid-Materials; 3d Printing, Nanofibers; Thin Films; Microcapsules; Bio-Nano and Bio-Material Interactions.

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Maciej Sznajder is a scientific co-worker at the Institute of Space Systems at the German Aerospace Center (DLR) in Bremen. He studied computational astrophysics at the University of Zielona Góra, Poland where he also obtained his first PhD in theoretical physics in 2013. And second, in the engineering field, was obtained at the Bremen University in 2016.

Research areas: Radiation analysis and testing; Aging mechanisms of materials used in space industry; Theoretical aspects of radiation interaction with matter; Computational physics and astrophysics; Data analysis.

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Patric Seefeldt is a 39 years old mechanical engineer with a diploma (RWTH Aachen 2010) and a PhD (University of Bremen 2018). As deputy head of the Mechanics and Thermal Systems Department (since 2016) and head of the Material Aging Group (since 2019) at DLRs' Institute of Space Systems, he is pursuing research in the field of innovative applications of new materials for space technologies.

