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SOLAR TECHNOLOGIES
go HYBRID

13th SolTech Conference

Sept. 25 – 27, 2024

Nuremberg

FAU
Friedrich-Alexander-Universität
Erlangen-Nürnberg

13th SolTech Conference

Sept. 25 – 27, 2024

Nuremberg

Conference Schedule (status: Sept. 15, 2024 - subject to change)

Wednesday, Sept. 25, 2024		
12:00-13:00	**Registration & Snacks**	
Session 1 / Chair: D. Guldi		
13:00	D. Guldi	Opening
13:15	G. Scholes (Princeton)	Coherence phenomena and quantum-like states
14:00	L. Kroh (BT)	Spectral Signatures and Kinetics of Y6 Aggregates and Disordered Phase via Absorption Spectroscopy
14:20	S. Krishna (FAU)	Pushing the limits towards long-lived charge-separation in Ru(II)phthalocyanine subporphyrazine conjugates
14:40	W. Tian (LMU)	Microplastic degradation and carbon engineering from biomass
15:00 - 15:30	**Coffee Break**	
Session 2 / Chair: T. Clark		
15:30	S. Santra (TUM)	Bismuth Single Atom-Based Model Catalysts - A Strategic Intervention to Control CO2RR Selectivity
15:50	A.Halkic/M. Weber (WÜ)	From N_2 activation to nitrogen containing compounds: the role of borylenes
16:10	L. Kumar (BT)	Solution Processed Cu_2ZnSnS_4 (CZTS) for Photocatalytic Hydrogen Evolution in Visible Range
16:30	O. Ferreira (Uberlandia/LMU)	Development of Electrocatalysts for Conversion of CO_2 into Fuels at Industrially Relevant Conditions
16:50	M. Kestler (LMU)	Carrier lattice interactions in photocatalytic bismuth oxyiodide
17:10	F. Negri (Bologna)	Decoding the optoelectronic properties of conjugated diradicals: insights from quantum-chemical modeling
18:00	**Session End**	

Thursday, Sept. 26, 2024		
Session 3 / Chair: NN		
08:30	K. Moth-Poulsen (PUC)	Solar energy conversion and energy storage materials
09:15	W. Kaiser (TUM)	Machine Learning the Dynamics of Energy Materials
09:35	C. Brabec (FAU)	Discovering Optimized Materials and Processes for Perovskite PV Technologies
09:55	K. Sailer (StMWK)	TBC
10:05-10:35	**Coffee Break**	
Session 4 / Chair: NN		
10:35	Y. Yao (BT)	Adapting Explainable Machine Learning to Study Mechanical Properties of Two-Dimensional Hybrid Halide Perovskites
10:55	J.L. Greenfield (WÜ)	Switching It Up: Enhancing the Photochromic Behavior of Imines
11:15	Le Du (TUM)	Pt-CN loaded hydrogel films for H_2 evolution system
11:35	B. Esser (Ulm)	Organic Electrode materials for next-generation batteries
12:20-13:30	**Lunch Break**	
Session 5 / Chair: NN		
13:30	Student Highlights	F. Gröbmeyer (LMU), Y. Bo (FAU), D. Dankert (TUM), H. Hoh (JMU), C. Greve (BT) - 6 min. each
14:00	L. Elbaz (Bar-Ilan)	Development of high surface area metal oxide aerogels for OER
14:45	M. Kuhn (BT)	Tuning methylammonium lead iodide crystallization with additives: a combined approach of microscopy, spectroscopy and machine learning
15:10	L. Kreimendahl (WÜ)	Diffusion Generative Models for Designing Efficient Singlet Fission Dimers

15:30 - 16:00	**Coffee Break**	- 6 -

Session 6 / Chair: NN		
16:00	N. Jux (FAU)	Fusing porphyrins to polycyclic aromatic hydrocarbons
16:20	S. Garain (WÜ)	The Delayed Box: Biphenyl-bisimide Cyclophane, a Supramolecular Nano-environment for Efficient Generation of Delayed Fluorescence
16:40	F. Zysman-Colman (St. Andrews)	New frontiers in photocatalyst design and photocatalysis

Postersession 1 / Hall Ground floor	
17:30 - 20:00	**Poster Session and Get Together**

Friday, Sept. 27, 2024

Session 7 / Chair: NN

08:30	F. Toma (Hereon, Teltow)	Closing the carbon cycle: how to make sustainable fuels and products
09:15	K. Gubanov (FAU)	The role of molecular di-oxygen in phenazine-TCNQ charge transfer complexes: regeneration and hydrogen evolution
09:35	H. Übele (TUM)	Potential Pulsed CO_2 Reduction Reaction on Polycrystalline Copper Electrodes Studied with Operando Plasmonic Interface Analysis
09:55	I. Ivanovic (LMU)	High-pressure methodology for clarifying the PCET mechanisms in ground and excited states

Postersession 2 / Hall Ground floor

10:15 - 11:45	Posters , Coffee & Pastry

Session 8 / Chair: F. Würthner

11:45	G. Thomas (IISER, India)	Exciton and biexciton dynamics in semiconductor nanocrystals
12:30	R. Tykwinski (Univ. Alberta)	Acenes for Up- and Down-conversion
13:15	N.N.	Poster Awards, Closing Remarks
13:30 -14:30	Snacks & Goodbye	

Abstracts (in consecutive order)

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14:40	W. Tian (LMU)	Microplastic degradation and carbon engineering from biomass

COHERENCE PHENOMENA AND QUANTUM-LIKE STATES

Gregory D. Scholes[a]

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There are a rich variety of ways molecules can interact with each other and their environment, and the span of possible timescales—from femtoseconds to nanoseconds. It is desirable to develop experiments that to reveal another "layer" of information—beyond kinetics—to inform sophisticated theoretical models. I will discuss how observing vibrational wavepackets can serve as a molecular-scale probe to give insight into the reaction coordinate of electron transfer (ET) reactions. Valuable insights into electron trans-fer reactions have been established using Marcus theory. However, a complementary theoretical model explaining how vibrational wavepackets evolve during electron transfer reactions has not yet been established. I will describe a "quantum quench" model to address this gap. In the second part of the talk I will explain how to invert the paradigm that complexity diminishes quantum coherence, so that robust *quantum-like states* emerge from extremely large, unordered, complex systems [1]. I will demonstrate a proposition for the structure of those states, showing how classical systems can indeed mimic the superpositions of products that characterize quantum states.

[1] G. D. Scholes, Proc. R. Soc. A 480., 2295 (2024).

SPECTRAL SIGNATURES AND KINETICS OF Y6 AGGREGATES AND DISORDERED PHASE VIA ABSORPTION SPECTROSCOPY

D. Kroh[a,b], **X. Xu**[b], **T. Smith**[b] and **A. Köhler**[a]

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[b]*University of Melbourne, Ultrafast and Microspectroscopy Laboratories, School of Chemistry, VIC 3010, Melbourne, Australia*

Recent advancements in single-junction organic solar cells (OSCs) utilizing non-fullerene acceptors (NFAs) have significantly increased power conversion efficiencies (PCEs) to over 19%. This remarkable progress is largely attributed to the introduction of the "Y-series" NFAs, with Y6 being the most notable example. Motivated by these achievements, numerous research groups are investigating the relationship between film morphologies and their exceptional optoelectronic properties, especially when blended with the donor material PM6.

In our study, we employed temperature-dependent steady-state UV-Vis absorption and photoluminescence spectroscopy combined with Franck-Condon analysis to identify the spectral signatures of two types of aggregates and the disordered phase of Y6 in solution. We observed that all three phases are also present in neat Y6 films and blend films with PM6. Through transient absorption measurements, we further explored the excitation kinetics and transient absorption spectral signatures of these phases, providing deeper insights into their behavior.

PUSHING THE LIMITS TOWARDS LONG-LIVED CHARGE SEPARATION IN RUTHENIUM (II) PHTHALOCYANINE-SUBPORPHYRAZINE CONJUGATES

S. Krishna[a], **E. Cañizares-Espada**[b], **D. Guzmán**[b], **Y. Bo**[a], **T. Clark**[c], **T. Torres**[b], **M. S. Rodriguez-Morgade**[b], **D. M. Guldi**[a]

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In the context of solar energy conversion, porphyrinoids-based donor-acceptor (D-A) systems are widely investigated due to their tunable optoelectronic properties, rapid energy/electron transfer capabilities, and the ability to produce long-lived charge-separated states.[1] Porphyrinoids like ruthenium(II) phthalocyanines (RuPcs) are often used in D-A arrays as they afford stable and strongly coordinated assemblies and promote rapid charge separation.[2] Subporphyrazines (SubPzs), a class of contracted porphyrinoids, exhibit optoelectronic properties that can be tailored through functionalizations.[3] Here, we present a series of RuPc-SubPz conjugates, which exhibit energy and electron transfer processes based on the SubPz design, highlighting their potential in the field of artificial photosynthesis.

[1] C. G. Claessens et al, *Chem. Rev.* **2014**, *114,* 2192–2277.

[2] M. S. Rodríguez-Morgade et al, *J. Am. Chem. Soc.* **2006**, *128,* 15145-15154.
[3] E. Caballero et al, *Chem. Eur. J.* **2014***, 20,* 6518–6525.

Microplastic degradation and carbon engineering from biomass

<u>W. Tian</u>[a,b], S. Wang[b] and E. Cortés[a]

[a] *Nanoinstitute Munich, Faculty of Physics, Ludwig-Maximilians-Universität München, 80539, Munich, Germany*
[b] *School of Chemical Engineering, The University of Adelaide, SA5005, Adelaide, Australia*

In tackling microplastic pollution and advancing green hydrogen production, this study reveals a tandem catalytic microplastic degradation-photocatalytic hydrogen evolution reaction (MPD-HER) process using hierarchical porous carbon nitride-supported single-atom iron catalysts.[1] Through hydrothermal-assisted Fenton-like reactions, we accomplish near-total ultrahigh-molecular-weight-polyethylene degradation into C_3-C_{20} organics, and a subsequent hydrogen evolution of 42 µmol h^{-1} under illumination, outperforming most existing plastic photoreforming methods. This tandem MPD-HER process not only provides a scalable and economically feasible strategy to combat plastic pollution but also contributes to the hydrogen economy, with far-reaching implications for global sustainability initiatives. Besides, we will also discuss the engineering of carbon-based catalysts from different flaky or acicular plant biomass to understand biomass structures and their effects on carbon properties and applications in environmental and energy area.[2]

[1] J. Lin, K. Hu, Y. Wang[1], W. Tian* *et al*, Nat Com, (2024, NCOMMS-24-26541-T, under revision).
[2] W. Tian et al, Nat Com, (2024, NCOMMS-24-38231, under review).

Session 2 / Chair: T. Clark		
15:30	S. Santra (TUM)	Bismuth Single Atom-Based Model Catalysts - A Strategic Intervention to Control CO2RR Selectivity
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BISMUTH SINGLE ATOM-BASED MODEL CATALYSTS - A STRATEGIC INTERVENTION TO CONTROL CO2RR SELECTIVITY

Saswati Santra[a,b,*], **Verena Streibel[a,b]**, **Laura Wagner[a,b]**, **Ningyan Cheng[c]**, **Pan Ding[a,b]**, **Guanda Zhou[a,b]**, **Elise Sirotti[a,b]**, **Ryan Kisslinger[a,b]**, **Tim Rieth[a,b]**, **Siyuan Zhang[c]** and **Ian D. Sharp[a,b,*]**

[a]*Walter Schottky Institute, Technical University of Munich, Germany*
[b]*Physics Department, TUM School of Natural Sciences, Technical University of Munich, Germany*
[c]*Max Planck Institute for Iron Research, Düsseldorf, Germany*

The CO_2 reduction reaction (CO2RR) has shown promise for producing C1-based feedstocks, including formic acid, CO, and syngas, under ambient conditions. Yet, achieving precise control over the reaction pathway to tune product selectivity remains a significant challenge. Single-atom catalysts (SACs) offer potential due to their tunable coordination environments, which may facilitate tuned catalytic activities and selectivities, while also offering insights into structure-activity relationships. Among active elements, bismuth (Bi) is a well-known CO2RR catalyst and primarily produces formic acid in aqueous electrolytes. Recently, it has also been reported for CO generation. Although these results indicated that different Bi coordination environments might be responsible for different product selectivity these products stem from dissimilar catalytic systems. To exclude other influences on selectivity, in our work, we exploit the well-defined atomic structure and tunable coordination environment of Bi-based single-atom catalysts (SACs) embedded in the same carbon-based host material. We show that the coordination environment of a single metallic species can be used to tune product selectivity. Since the versatility of a single CO2RR catalyst system for producing two different major products has rarely been reported, our work opens up a new direction for tuning the CO2RR C1 product selectivity using SACs. In the future, assembly of these atomically-defined catalysts with light absorbing elements offers

potential for steering product distributions from artificial photosystems.

FROM N₂ ACTIVATION TO NITROGEN CONTAINING COMPOUNDS: THE ROLE OF BORYLENES

<u>A. Halkić</u>[a], <u>M. Weber</u>[a], T. Kunz[a] and H. Braunschweig[a]

[a] Institute for Inorganic Chemistry and Institute for Sustainable Chemistry & Catalysis with Boron (ICB), Julius-Maximilians-Universität Würzburg, Am Hubland, 97074 Würzburg, Germany.

For over a century, the ability to activate dinitrogen was limited to the transition metals[1] and lithium[2]. The astounding potential of borylenes in the activation of dinitrogen, was first demonstrated by Braunschweig and coworkers in 2018 and can thus be regarded as main-group-metallomimetic.[3] Singly Lewis-base-stabilized borylenes turned out to be the most suitable for the activation of dinitrogen, forming bis(borylene) complexes with end-on bridging N_2- and N_4-units, as well as terminal borylene-diazenide complexes with suitable silyl trapping agents.[4] Herein we report the synthesis of a range of new borylene-N_2/N_4 complexes.[4,5] Further functionalization and/or cleavage of the activated N_2-unit was achieved through simple chemical conversions with readily available chemicals. The resulting products are of great interest to both research and industry, due to the high demand for synthetic nitrogen-containing building blocks.[4-6]

[1] B. A. MacKay, M. D. Fryzuk, Chem. Rev. 104, 2, 385–402 (2004). [2] D. H. Gregory, Coord. Chem. Rev. 215, 301–345 (2001). [3] M.-A. Légaré, C. Pranckevicius, H. Braunschweig, Chem. Rev. 119, 14, 8231–8261 (2019). [4] A. Gärtner, H. Braunschweig et al., J. Am. Chem. Soc. 145, 14, 8231–8241 (2023). [5] M. Rang, H. Braunschweig et al., J. Am. Chem. Soc. 146, 16, 11048–11053 (2024). [6] M. Weber, H. Braunschweig et al., Angew. Chem. Int. Ed. 63, e202402777 (2024).

SOLUTION PROCESSED Cu2ZnSnS4 (CZTS) FOR PHOTOCATALYTIC HYDROGEN EVOLUTION IN VISIBLE RANGE

L. KUMAR, M. Goel, T. P. Gujar, M. Thelakkat*

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Efficient, scalable, and affordable sunlight-driven water-splitting systems are essential for widespread solar hydrogen production as a renewable energy source. Cu_2ZnSnS_4 (CZTS) is gaining prominence due to its favorable electrical and optical properties, enabling its utilization in photocatalysis, photovoltaic devices, and electrocatalysis. This study utilizes a direct dip-coating method to fabricate porous CZTS thin films on various substrates. The procedure involves a sol-gel precursor comprising of metal salts and thiourea dissolved in methanol, followed by sulfurization under a nitrogen and hydrogen environment. To create a p-n heterojunction, a conjugated n-type perylene dye is vapor deposited onto CZTS layer followed by platinum sputtering onto hybrid films to generate catalytic surface. Analysis of the resultant films are performed using UV-Vis, Raman & Ultraviolet photoelectron spectroscopy, X-ray diffraction and scanning electron microscopy. The photocatalytic hydrogen evolution performance is subsequently assessed. CZTS thin films on molybdenum-coated substrates demonstrate improved efficiency of dye degradation and hydrogen evolution under visible light.

DEVELOPMENT OF ELECTROCATALYSTS FOR CONVERSION OF CO2 INTO FUELS AT INDUSTRIALLY RELEVANT CONDITIONS

Gonçalves J. Marrenjo[a], Mateus J. Tomas[a], Cleiton Policarpo[a] and Osmando F. Lopes[a]

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The electrochemical CO_2 reduction reaction (CO_2RR) into value-added products such as HCOOH and CO represents a promising technology to mitigate climate change and promote energy sustainability. Sn, Bi, and Zn electrocatalysts exhibit satisfactory selectivity for CO_2 conversion into HCOOH and CO, respectively. However, this process faces several drawbacks for a commercialization, such as low stability (< 50 h) and low current density (<30 mA cm^{-2}). In our group, we have been investigating different strategies using electrochemical flow-cell and Sn, Bi and Zn-based electrocatalysts to overcome these challenges. We demonstrated the amino functionalization of ZnO improved its CO_2RR performance delivering a current density of -130 mA.cm^{-2}, with a Faradaic efficiency exceeding 80% at -1.2 V *vs* RHE and a stability under 100h of operation. We also investigated the effect of SnO_2 and $Bi_2O_2CO_3$ morphology on the CO_2RR, we observed the nanosheets morphology resulted in the best performance reaching current densities higher than -200 mA.cm^{-2} with a selectivity for HCOOH exceeding 90%.

[1] F. Liu *et al*, Chem. Eur. J. Vol. 30, e202303711 (2024).

CARRIER LATTICE INTERACTIONS IN PHOTOCATALYTIC BIOI:

M. F. Kestler[a,b], K. C. Woo[b], J. W. X. Lim[b], L. M. Prins[a],

Z.-H. Loh[b] and J. Feldmann[a]

[a]*Chair for Photonics and Optoelectronics, Nano-Institute Munich and Department of Physics, Ludwig-Maximilians-Universität (LMU), Königinstr. 10, 80539 Munich, Germany*
[b]*School of Chemistry, Chemical Engineering and Biotechnology, and School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore 637371, Singapore*

Bismuth oxyiodide (BiOI) is a polar and indirect semiconductor, which is well known to efficiently drive photocatalytic reactions such as water splitting and oxygen reduction. After the recent observation of optically induced coherent phonons in BiOI [1], strong carrier phonon coupling is expected to modify further electronic properties of BiOI. As an example, a long-lived transient absorption signal has been related to the existence of polarons in this catalytic system.

To investigate the properties of such polarons we employed time-resolved photoemission electron microscopy (TR-PEEM). This unique pump-probe method offers the possibility to monitor the electronic dispersion as a function of time. We observe a flattening and energetic drop of the conduction band structure in accordance with theoretical predictions by Fröhlich.

[1] Rieger, S. et al. "Optically Induced Coherent Phonons in Bismuth Oxyiodide (BiOI) Nanoplatelets." Nano Letters 21, 7887 (2021).

DECODING THE OPTOELECTRONIC PROPERTIES OF CONJUGATED DIRADICALS: INSIGHTS FROM QUANTUM-CHEMICAL MODELING

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In recent decades, open-shell conjugated organic molecules have emerged as a novel class of materials, holding significant promises across various fields: organic electronics, photonics, spintronics and quantum devices.[1] I will describe the essential optoelectronic properties of conjugated chromophores exhibiting diradical character, some of which have revealed complete absence of emission, showcasing outstanding photo-thermal conversion capabilities.[2] Unexpected luminescent behavior has been uncovered, instead, for some paraquinodimethane derivatives.[3] I will also overview our recent investigations on charged species derived from conjugated diradicals, playing crucial roles in organic semiconductors and energy storage substrates. Although the pool of molecules stabilizing both anions and cations remains limited, conjugated diradicals can circumvent this limitation.[4]

[1] Dong, S.; et al.; J. Mater. Chem. C 10, 2431–2449 (2022).
[2] Ji, Y.; et al.; Angew. Chem. Int. Ed. Engl. 62, e202311387 (2023).
[3] Punzi, A.; et al.; J. Am. Chem. Soc. 145, 20229–20241 (2023).
[4] Mori, S.; et al.; Angew. Chem. Int. Ed. Engl. 61, e202206680 (2022).

Session 3 / Chair: NN		
08:30	B. Esser (Ulm)	Organic electrode materials for next-generation batteries
09:15	W. Kaiser (TUM)	Machine Learning the Dynamics of Energy Materials
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09:55	K. Sailer (StMWK)	TBC

ORGANIC ELECTRODE MATERIALS FOR NEXT-GENERATION BATTERIES

B. Esser[a]

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In face of the climate change there is a strong and growing demand for the storage of renewable energies. Organic electrode materials have attracted great interest for next-generation batteries, as they can be prepared from renewable, sustainable or less-limited resources, they are easy to recycle as well as potentially safer and cheaper to produce. Both p- and n-type organic materials with reversible redox processes can be used, often based on π-systems, furnishing different types of cell configurations.[1,2] In this talk design principles and examples of organic battery electrode materials and their application in all-organic and multivalent metal full cells as well as in a photo battery will be discussed.

[1] B. Esser, F. Dolhem, M. Becuwe, P. Poizot, A. Vlad, D. Brandell, *J. Power Sources* **2021**, *482*, 228814
[2] B Esser, *Org. Mater.* **2019**, *01*, 063–070.

Machine Learning the Dynamics of Energy Materials

Waldemar Kaiser[a], Takeru Miyagawa[a], Frederico Delgado[a], Namita Krishnan[a], Manuel Grumet[a], David A. Egger[a]

[a]Department of Physics, TUM School of Natural Sciences, Technical University of Munich, James-Franck Str. 1/I, 85748 Garching, Germany

An accurate description of atomic motions can provide fundamental insights into the structure-property relationships and the stability of energy materials at finite temperatures. We leverage machine-learning molecular dynamics (MLMD), trained on-the-fly on ab initio molecular dynamics simulations, to study various dynamical properties of energy materials. First, we investigate the motion of ions and ionic point defects within solid-state ion conductors [1]. Specifically, we demonstrate the accuracy of ML-generated force fields in describing the motion of ions in various systems, all of which include vibrational anharmonicities. Second, we examine the impact of ionic dynamics on the electronic properties of halide perovskite surfaces to identify the dynamic nature of surface states. Both studies demonstrate the potential of MLMD to accurately capture atomic motions for an improved understanding of dynamical properties of energy materials.

[1] T. Miyagawa, et al. J. Mater. Chem. A. (2024),12, 11344-11361.

Discovering Optimized Materials and Processes for Perovskite PV Technologies

Christoph J. Brabec

Institute of Materials for Electronics and Energy Technology (i-MEET), Department of Materials Science and Engineering, FAU, Martensstrasse 7, 91058 Erlangen & Helmholtz-Institute Erlangen-Nürnberg (HI ERN), Forschungszentrum Jülich, Immerwahrstrasse 2a, 91058 Erlangen, Germany

Perovskite photovoltaics poses a multi-objective optimization problem in a large multi-dimensional parameter space. Massive progress was achieved in developing methods to accelerate solving such complex optimization tasks. We have demonstrated that the combination of Gaussian Process Regression (GPR) and Bayesian Optimization (BO) are most efficient in predicting new materials, identify optimized processing conditions or invent alternative device architectures in larger parameter rooms. For a 4 dim space (e.g. solvent, donor-acceptor ratio, spin speed, concentration) with about 1000 variations in a 10% grid space, 30 samples are sufficient to find the optimum. For 5 & 6 dimensional spaces, the possible variations go into the millions – still, the autonomous optimization strategies are working with a surprising low number of experiments. Our automated lines, being operated in an autonomous optimization mode, were able to identify globalized optima within several hundred´s of experiments. That raises the question whether these large material spaces as well hold the promise for discoveries. We extended the BO concept towards the discovery of new molecules that can be integrated into the device optimization cycle. The research campaign found molecular semiconductors that had not been published before but yielded performance values bypassing the current state of the art materials.

Session 4 / Chair: NN		
10:35	Y. Yao (BT)	Adapting Explainable Machine Learning to Study Mechanical Properties of Two-Dimensional Hybrid Halide Perovskites
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11:15	Le Du (TUM)	Pt-CN loaded hydrogel films for H_2 evolution system
11:35	K. Moth-Poulsen (PUC)	Solar energy conversion and energy storage materials

ADAPTING EXPLAINABLE MACHINE LEARNING TO STUDY MECHANICAL PROPERTIES OF TWO-DIMENSIONAL HYBRID HALIDE PEROVSKITES

Yuxuan Yao[a,b], **Dan Han**[c,d], **Hubert Ebert** [d] **and Harald Oberhofer**[b]

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[b]*University of Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany*
[c]*University of Birmingham, Edgbaston, Birmingham, B15 2TT, United Kingdom*
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The fast increase of power conversion efficiency (PCE) and low-cost preparation of lead-based halide perovskite photovoltaics are of great interest in optoelectronic devices. 2D hybrid organic and inorganic perovskites (HOIPs) have been used as capping layers on top of 3D perovskites to increase the stability and PCE. In our work, we utilize explainable machine learning (ML) techniques to accelerate the in silico prediction of elasticities of 2D perovskites, as indicated by their Young's moduli. Our ML models allow us to distinguish between stiff and non-stiff HOIPs and to extract the materials' features most strongly influencing the Young's modulus. The Pb-halogen-Pb bond angle emerges as the dominant physical feature with an inverse correlation to the structural non-stiffness. Furthermore, the cations' steric effect index (STEI) was found to yield rough estimates of non-stiffness. Finally, the deformation of the octahedra affects the mechanical properties, allowing us to perform transferability test from single layered to multi-layered 2D perovskites.

Switching It Up: Enhancing the Photochromic Behavior of Imines

Jake L. Greenfield [a,b]

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[b] Center for Nanosystems Chemistry (CNC), Universität Würzburg, 97074 Würzburg, Germany

Molecules and materials comprised of dynamic-covalent imine bonds display many desirable properties, including stimuli-responsiveness, recyclability, and effortless preparation, among others. One frequently overlooked property of imines is their photochromism due to its historically poor performance compared to other photoswitches. Recently, we found a strategy for improving these photoswitching properties,[1] achieving quantitative conversion to the metastable state using visible light and thermal half-lives over 19 hours. This now opens new opportunities[2] including exploring their use as Molecular Solar Thermal (MOST) materials.

[1]   J. Wu, L. Kreimendahl, S. Tao, O. Anhalt, J. L. Greenfield, *Chem. Sci.* **2024**, *15*, 3872–3878.
[2]   J. Wu, J. L. Greenfield, *J. Am. Chem. Soc.* **2024**, *146*, 20720–20727.

PT-CN LOADED HYDROGEL FILMS FOR H_2 EVOLUTION SYSTEM

M. P. Le Dû[a], **D. Kosbahn**[a], **T. Baier**[a], **J. Reitenbach**[a],**Q. Zhong**[b], **A. Vagias**[c], **R. Cubitt**[c], **N. Chalagain**[d], **K. Shankar**[d], **H. Übele**[e], **K. Krischer**[e], **P. Müller-Buschbaum**[a]

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Platinum (Pt) loaded carbon nitride (CN) is a promising photocatalyst under visible light for green hydrogen (H_2) production. We aim to develop this system in a thin polymer film to make it industrially scalable. The Poly(N-isopropylacrylamide) (PNIPAM) hydrogel is used as a host matrix and water storage medium to facilitate homogeneous dispersion of the catalytic centers. The hybrid film's vertical distribution and inner microstructure are studied under *operando* conditions with time-of-flight neutron reflectometry (ToF NR) and grazing incidence small angle neutron scattering (GISANS). The resulting H_2 produced is measured by gas chromatography.

SOLAR ENERGY CONVERSION AND ENERGY STORAGE MATERIALS

K. Moth-Poulsen[a, b, c, d]

ᵃPolytechnic University of Catalunya ᵇ Catalan Institution for Research and Advanced Studies, ᶜInstitute of Materials Science of Barcelona, ᵈChalmers University of Technology, Gothenburg, Sweden

Since the beginning of civilization, humanity has built houses to sustain comfortable living conditions throughout the seasons. In our modern society, about 50% of the total energy consumption is used for heating and cooling. Growing demands for thermal management in many different sectors, from electronics to housing, inevitably mean increased energy consumption.

In this lecture I will present how we are working on developing molecular materials that capture, store, and release both solar and ambient heat without creating any emissions. These molecular solar thermal systems (MOST) are based on molecular photoswitches that absorb light and convert it into stored chemical energy, that can be released on demand[1-6] (Fig.1). The MOST energy system operates through different principles than traditional solar thermal and can be introduced into compact energy capture and release devices. Recently, the first example of integration of the energy storage system with photovoltaics, and in electric power generation devices was published[7-8].

[1]   Z. Wang, et al. Energy and Environmental Science, 2019, 12, 187-193. (cover) [2] M. Mansø, et al. Nature Communications 2018, 9:1945. [3] A. Dreos et al. Energy and Environmental Science 2017, 10, 728-734. (cover) [4] A. U. Petersen, Advanced Science, 2019, 1900367. [5] Z. Zhang et al. J. Am. Chem. Soc. 2020, 142, 28, 12256–12264. [6] Z. Wang, Joule 5(12), 3116-3136, 2021 [7] Z. Wang, et al. Joule 2024 (accepted)

Session 5 / Chair: NN		
13:30	Student Highlights	F. Gröbmeyer (LMU), Y. Bo (FAU), D. Dankert (TUM), H. Hoh (JMU), C. Greve (BT) - 6 min. each
14:00	L. Elbaz (Bar-Ilan)	Development of high surface area metal oxide aerogels for OER
14:45	M. Kuhn (BT)	Tuning methylammonium lead iodide crystallization with additives: a combined approach of microscopy, spectroscopy and machine learning
15:10	L. Kreimendahl (WÜ)	Diffusion Generative Models for Designing Efficient Singlet Fission Dimers

FLASH TALKS (6 MINUTES)

F. Gröbmeyer (LMU)	*Interferometric Scattering in Battery Materials*
Y. Bo (FAU)	*Intramolecular down- and up-conversion in dimeric tetracene complexes centered via Pt(II) and Pd(IV)*
D. Dankert (TUM)	*Investigations on the optoelectronic properties of compounds bearing small homoatomic clusters of the tetrel elements*
H. Hoh (JMU)	*Guest-Mediated Modulation of Photophysical Pathways in a Coronene Bisimide Cyclophane*
C. Greve (BT)	*GIWAXS studies of 2D Ruddlesden-Popper Perovskites for Photomemristors applications*

NB: Each flash talk will also be presented as poster in one of the two poster sessions

DEVELOPMENT OF ADVANCED HIGH SURFACE AREA METAL OXIDE AEROGELS FOR OER

L. Elbaz

Chemistry Department, Bar-Ilan University, Ramat-Gan 5290002, Israel

The need for sustainable energy storage is undisputable, and green hydrogen seem to be one of the most promising options to do so. Yet, the price of water electrolysis to produce green hydrogen is still too high to make it competitive with existing solutions. To tackle this issue, more and more non-precious metal OER catalyst have been developed in recent years. Most notably is the family of mixed nickel-iron oxyhydroxides (NiFeOOH), which show promising performance in alkaline media. One challenge that remains is to increase the NiFeOOH surface area, and by that the electrochemically active site density (EASD). In this regard, one class of materials that has been attracting the attention of materials' scientists in recent years are aerogels. In this talk I will preset our work on NixFeyMzOOH aerogels. These aerogels show much higher active site utilization and overall increase in mass activity for OER when compared to other NiFeOOH derived materials. They were tested for their activity and to the best of our knowledge these are the first aerogel materials that catalyze OER themselves, rather than being used merely as support material. The catalytic activity depends largely on the metals' ratio, pore size distribution and total surface area. I will explain their activity from an experimental and theoretical perspectives and present the state-of-the-art performance for this category of catalysts in AEMWEs.

TUNING METHYLAMMONIUM LEAD IODIDE CRYSTALLIZATION WITH ADDITIVES: A COMBINED APPROACH OF MICROSCOPY, SPECTROSCOPY, AND MACHINE LEARNING

A. Meike Kuhn [a], B. Milan Harth [b], C. Alessio Gagliardi [b] and D. Eva M. Herzig[a]

[a]Dynamik und Strukturbildung - Herzig Group, Universitätsstraße 30, 95447 Bayreuth, Germany
[b] Simulation of Nanosystems for Energy Conversion, Technische Universität München, Hans-Piloty-Str. 1, 85748 Garching b. München

The interest in perovskite materials has increased in the last years due to progress made in a wide range of perovskite applications. Thereby, the crystallization process plays a fundamental role in determining the final properties of the perovskite layer. The use of additives offers a promising approach to modulating crystal growth and thereby determining the final properties. Techniques like microscopy and spectroscopy can help analyze this crystallization process in a time-resolved manner. However, due to the production of large data sets, machine learning is useful for predicting these crystallization phenomena.

In this study, we focused on the crystallization of methylammonium lead iodide (MAPbI3) by introducing a tailored supramolecular additive (SBBA) to influence perovskite formation. Using spectroscopy and microscopy techniques, we analyzed the impact of the additive on crystal morphology and optical properties. A machine learning model was also developed to predict spectroscopic signals from microscopic images, to allow access to information on a smaller nanoscale by microscopy.

DIFFUSION GENERATIVE MODELS FOR DESIGNING EFFICIENT SINGLET FISSION DIMERS

L. Kreimendahl[a], **M. Karnaukh**[a] **and M. I. S. Röhr**[a,b]

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[b]*Center for Nanosystems Chemistry, Julius-Maximilians-Universität Würzburg, Theodor-Boveri Weg, 97074 Würzburg, Germany*

Diffusion generative models, a class of machine learning techniques, have shown remarkable promise in materials science and chemistry by enabling the precise generation of complex molecular structures. We propose a novel application of these models to stabilize reactive molecular structures identified through quantum mechanical screening, focusing on the design challenge of Singlet Fission (SF), which is crucial for advancing solar cell efficiency beyond theoretical limits. Although theoretical chemistry predicts intermolecular arrangements with enhanced SF coupling, practical implementation faces challenges due to discrepancies between favorable and stabilized structures. To address this, we introduce a two-step strategy combining quantum mechanical screening for identifying optimal arrangements and diffusion generative models for predicting stabilizing linkers. Our approach, demonstrated through a case study on Cibalackrot dimers, shows efficacy in enhancing SF efficiency by stabilizing the desired molecular arrangements.

Session 6 / Chair: NN		
16:00	N. Jux (FAU)	Fusing porphyrins to polycyclic aromatic hydrocarbons
16:20	S. Garain (WÜ)	The Delayed Box: Biphenyl-bisimide Cyclophane, a Supramolecular Nano-environment for Efficient Generation of Delayed Fluorescence
16:40	F. Zysman-Colman (St. Andrews)	New frontiers in photocatalyst design and photocatalysis

FUSING PORPHYRINS TO PAHS

N. Jux[a], C. Oleszak[a] and F. Bozinovic[a]

aI Friedrich-Alexander-Universität Erlangen-Nürnberg, Department of Chemistry & Pharmacy and Interdisciplinary Center for Molecular Materials

Fusing porphyrins to various polycyclic aromatic hydrocarbons is an excellent strategy to expand the π-system of the porphyrin and add functionality.[1-2] Thus, new chromophores are obtained which possess, among other interesting qualities, red-shifted UV/vis absorptions.
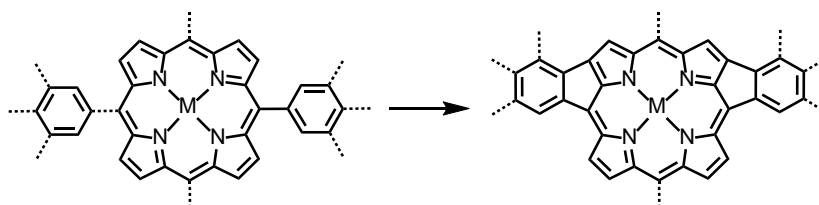
We present our approach to π-extended fused porphyrins via Scholl oxidation of meso-positioned aryl groups to the core.[3,4]

1. Roznyatovskiy VV, Leeb CH, Sessler JL. *Chem. Soc. Rev.* **2013**, *42*, 1921-1933.
2. Lewtak JP, Gryko, DT. *Chem. Commun.* **2012,** *48*, 10069-10086.
3. Martin MM, Oleszak C, Hampel F, Jux N. *Eur. J. Org. Chem.* **2020**, *40*, 6578-6762.
4. C. Oleszak, P. R. Schol, C. L. Ritterhoff, M. Krug, M. M. Martin, Y. Bo, B. Meyer, T. Clark, D. M. Guldi, Norbert Jux Angew. Chem. Int. Ed., accepted; DOI: 10.1002/anie.202409363

The Delayed Box: Biphenyl-bisimide Cyclophane, a Supramolecular Nano-environment for Efficient Generation of Delayed Fluorescence

S. Garain[a], K. Shoyama[b], L. M. Ginder[a], M. Sárosi[a], F. Würthner[a,b*]

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The burgeoning field of host-guest chemistry recently created immense attention in supramolecular chemistry due to their strong binding affinity and selectivity.[1] Moreover, cyclophane hosts recently started blossoming due to their unique molecular design and functional relevance in sensing and catalysis. However, triplet-induced functional properties are still unknown in this scientific realm and remain a holy grail. In this context, we propose a strategy for efficient delayed fluorescence emission in a dilute solution state using a non-covalent approach via supramolecular nano–environment formation. We aim to create supramolecular nanocavity for triplet exciton stabilization by reducing vibrational dissipation and lowering the singlet-triplet energy gap for efficient delayed fluorescence emission.[2] We elegantly entrench the design to alleviate the scenario using a novel small biphenyl bisimide-derived cyclophane, an electron-deficient and efficient triplet-generating host. We intend to form an emissive charge-transfer (CT) state close to the triplet level of the biphenyl bisimide upon encapsulating carbazole-derived guest inside the nanocavity of cyclophane. The experimental results of host-guest studies manifest high association constants up to 10^4 M^{-1}, which help in strong inclusion complex formation, prerequisites for emissive CT state evolution, and triplet-state stabilization in a diluted solution. According to our hypothesis, we realize tunable delayed fluorescence emission from carbazole-encapsulated biphenyl bisimide cyclophane in methylcyclohexane carbon tetrachloride solution via non-covalent supramolecular strategy with significantly high quantum yield (QY) of up to 15.6 %. Further crystal structure analysis and solid-state photophysical study validate our hypothesis and elucidate the delayed fluorescence emission mechanism.

References:

[1] H. Uoyama, K. Goushi, K. Shizu, H. Nomura, C. Adachi, *Nature* **2012,** *492*, 234–238.

[2] P. Spenst, F. Würthner, *Angew. Chem. Int. Ed.* **2015**, *54*, 10165–10168.

EXCITON AND BIEXCITON DYNAMICS IN SEMICONDUCTOR NANOCRYSTALS

K. George Thomas

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Vithura, Thiruvananthapuram, 695551, India

Developing semiconductor systems for light energy harvesting and optoelectronic applications require an in-depth understanding of exciton and biexciton dynamics, as well as charge delocalization of photogenerated carriers. Compared to binary (II–VI and III–V) semiconductor nanocrystals (NCs), lead halide perovskite nanocrystals (PNCs) offer several notable advantages due to their defect tolerance. The first part of the talk will explore the dynamics of bound charge carriers in both binary semiconductor NCs and lead halide PNCs using time-resolved emission spectroscopy. Our findings reveal that trap depth plays a vital role in exciton dynamics in semiconductor quantum dots whereas the biexciton quantum efficiency in cesium lead bromide PNCs is influenced by the number of facets. As progressing from cube to rhombic dodecahedron, and further to rhombicuboctahedron PNCs, the biexciton quantum efficiency increases. This enhancement is primarily attributed to the increase in surface polarity as the number of facets increases, which reduces Coulombic interactions between charge carriers and suppresses Auger recombination. In the second part of the talk, I will present strategies to enhance electron delocalization in semiconductor heterostructures and vertex-oriented cube assemblies of perovskites.

[1] E. K. Vishnu *et al*, J. Phys. Chem. C 125, 25706-25716 (2021).
[2] E. M. Thomas *et al*, ACS Energy Lett. 7, 2856-2863 (2022).
[3] A. Garai *et al*, J. Am. Chem. Soc. 145, 13989-13999 (2023).
[4] E. K. Vishnu *et al*, J. Phys. Chem. C 128, 4373-4382 (2024).
[5] M. P. Varghese *et al*, J. Phys. Chem. C 128, 10945-10954 (2024).
[6] S. Bera *et al*, J. Am. Chem. Soc. 146, 20300-20311 (2024).
[7] T. Titus *et al*, Nano Lett. 24, 10434-10442 (2024).

Session 7 / Chair: NN		
08:30	F. Toma (Hereon, Teltow)	Closing the carbon cycle: how to make sustainable fuels and products
09:15	K. Gubanov (FAU)	The role of molecular di-oxygen in phenazine-TCNQ charge transfer complexes: regeneration and hydrogen evolution
09:35	H. Übele (TUM)	Potential Pulsed CO_2 Reduction Reaction on Polycrystalline Copper Electrodes Studied with Operando Plasmonic Interface Analysis
09:55	I. Ivanovic (LMU)	High-pressure methodology for clarifying the PCET mechanisms in ground and excited states

CLOSING THE CARBON CYCLE: HOW TO MAKE

SUSTAINABLE FUELS AND PRODUCTS

F. M. Toma[a,b,c]

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[c]*Lawrence Berkeley National Laboratory, 1 Cyclotron Road, 94720, Berkeley, CA, USA*

Fossil fuels are still our main source of carbon, which is not only utilized as one of the major sources of energy but as the main component of many materials around us.To aid future sustainable development, we need to reimagine the carbon cycle and create a circular economy by defossilizing the areas that will continue to need carbon. In our Institute, we address these issues by developing carbon alternatives based on solar fuels, and by improving our ability to reuse carbon through waste upcycling and synthetic design of renewable materials.

Here, we will share our most recent results on light driven H_2 production and CO_2 reduction. Examples will include devices based on Cu_2O [1] and ZnTe for CO_2 reduction, and perovskite photocathodes for both H_2 production and CO_2 reduction [2].

[1] G. Liu *et al*, Nature Energy. 6, 1124-1132 (2021).
[2] H. Choi *et al*, Advanced Sciences. 10(33), 2303106 (2023).

THE ROLE OF MOLECULAR DI-OXYGEN IN PHENAZINE-TCNQ CHARGE-TRANSFER COMPLEX REGENERATION & HYDROGEN EVOLUTION

K. Gubanov[a], **Y. Reva**[a], **D. Langford**[a], **F. Hampel**[a], **E. Franz**[a], **B. Watts**[b], **J. Libuda**[a], **D. M. Guldi**[a] **and R. H. Fink**[a]

[a]*Department of Chemistry and Pharmacy, Friedrich-Alexander-Universität Erlangen Nürnberg, Egerlandstraße 3, 91058 Erlangen, Germany*
[b]*Paul Scherrer Institute, Forschungsstraße 111, 5232 Villigen, Switzerland*

Organic charge-transfer complexes (CTC) are promising electrode materials in rechargeable lithium-ion batteries [1]. However, charge-trap states, induced by the structural defects within the CTC crystal lattice, lower the initial degree of charge transferred from the electron donor to acceptor molecules. Remarkably, di-oxygen-enriched environment regenerates the charge-transfer dynamics in the electron donor-acceptor complex of phenazine (PNZ)/7,7,8,8-Tetracyanoquinodimethane (TCNQ) crystals. Our findings demonstrate that the trap states within the CTC crystal are filled by electrons that stem from physisorbed di-oxygen. A unique example of organic semiconductor accepting electrons from the molecular oxygen to fill trap states opens a pathway to facilitate such material performance in organic-based batteries. In addition, regeneration of the charge-transfer state by di-oxygen results in substantially enhanced photo-stimulated hydrogen evolution from the respective CTC material.

[1] S. Lee *et al*, Energy Storage Mater., 462-469, 20 (2019).

POTENTIAL PULSED CO₂ REDUCTION REACTION ON POLYCRYSTALLINE COPPER ELECTRODES STUDIED WITH OPERANDO PLASMONIC INTERFACE ANALYSIS

H. Übele[a]**, M.J. Feil**[a] **and K. Krischer**[a]
[a]*Technische Universität München, TUM School of Natural Sciences, Physics Department, Nonequilibrium Chemical Physics, James-Franck Str. 1, 85748 Garching, Germany*

Cu and Cu_2O electrodes are the electrodes of choice for the reduction of CO_2 to hydrocarbons, such a methane, ethylene, or ethanol. However, they also are subject to fast degradation, inhibiting long-term operation under steady state conditions [1]. Here, we demonstrate that long-term stable nanostructured electrode morphologies can be obtained through potential pulsing when starting from merely polished polycrystalline Cu electrodes. Depending on the pulsing protocol, different product selectivities are realized, approaching those of manufactured nano-structured oxide-derived catalysts or Cu single crystal electrodes, respectively, but with a greatly enhanced longevity. The morphological changes are monitored in operando with plasmonic interface analysis, similar to differential Cyclic Plasmo-Voltammetry [2].

[1] Timoshenko, Janis, et al. Nature Catalysis 5.4 (2022): 259-267.
[2] Feil, Moritz J., et al. The Journal of Physical Chemistry C 127.40 (2023): 20137-20145.

HIGH-PRESSURE METHODOLOGY FOR CLARIFYING PCET MECHANISMS IN GROUND AND EXCITED STATES

D. Langford[a], Robin Rohr[b], Stefan Bauroth[a], Achim Zahl[b], Alicja Franke[c], Ivana Ivanović-Burmazović[c] and Dirk M. Guldi[a]

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[b]*Dept Chemistry & Pharmacy, FAU Erlangen-Nürnberg, 91058 Erlangen, Germany*
[c]*Department of Chemistry, Ludwig-Maximilian-Universität München, 81377 München, Germany*

We have elucidated the mechanism of excited-state proton-coupled electron transfer (PCET) for a model reaction, as depicted in Scheme 1 [1], using pressure-dependent measurements obtained through femtosecond and nanosecond resolved transient absorption spectroscopy (TAS) with a custom-built high-pressure detection cell. This unique study of excited-state PCET under high-pressure conditions has allowed us to demonstrate the effectiveness of variable pressure measurements in excited-state chemistry. Specifically, we were able to differentiate between stepwise and concerted PCET processes and introduce the concept of using pressure to modulate PCET mechanisms. This talk will also illustrate how our pressure-based approach can be broadly applied to PCET processes, including ground-state reactions, by employing techniques such as high-pressure NMR or stopped-flow methods.

[1] A. Pannwitz, O.S. Wenger, *Phys. Chem. Chem. Phys.*, 18, 11374 (2016).

Session 8 / Chair: F. Würthner		
11:45	G. Thomas (IISER, India)	Exciton and biexciton dynamics in semiconductor nanocrystals
12:30	R. Tykwinski (Univ. Alberta)	Acenes for Up- and Down-conversion
13:15	N.N.	Poster Awards, Closing Remarks

NEW FRONTIERS IN PHOTOCATALYST DESIGN AND PHOTOCATALYSIS

A. Eli Zysman-Colman[a]

[a]Organic Semiconductor Centre, EaStCHEM School of Chemistry, University of St Andrews, UK

In this talk I highlight some of our recent work in sustainable photocatalyst design, covering photocatalysts using Earth-abundant metals and those based on organic dyes. I will also discuss new innovations in photoreactor design.

ACENES FOR UP- AND DOWN-CONVERSION

Rik R. Tykwinski

Department of Chemistry, University of Alberta, Edmonton, Alberta, Canada T6G 2G2

Dimeric and oligomeric acenes (tetracene and pentacene)[1] are ideal to study photon energy conversion through studies that examine *intramolecular* SF (*i*SF)[2] and TTA-UC (*i*TTA-UC).[3] Among other advantages, photophysical studies in solution are greatly simplified for intramolecular systems since dilute solutions of the chromophore can be analyzed. Furthermore, the structure of the spacer linking two or more acenes can be used to define geometry, as well as the level of coupling between chromophores. Synthetic incorporation of specific spacers is used to tailor aspects of chromophore design, and, for example conjugated, non-conjugated, and organometallic spacers have been explored and compared.[1] Spacers can also be used to attach chromophores to surfaces in devices, as well as incorporate antennae such as subphthalocyanines to form conjugates that broaden the accessible absorption range. Our strategies for synthesis of selected acene oligomers will be presented in this talk, as well as the resulting characteristics of *i*SF and *i*TTA-UC.

[1] C. Hetzer, et al. *Chem. Eur. J.* 24, 8245–8257 (2018).
[2] P. M .Greißel, et al. *Angew. Chem. Int. Ed.* 63, e202315064 (2024).
[3] Y. Bo, Y. Hou, et al. *J. Am. Chem. Soc.* 145, 18260–18275 (2023).

Postersession 1 (Sept. 26, 2024 / 17:30 – 20:00)

P1: A Lab-Based NAP-XPS Setup to Probe Photoelectrochemical Interfaces under Working Conditions

Katarina S. Flashar[1], Ian D. Sharp[1], Barbara A. J. Lechner[2], Verena Streibel[1]
[1]Walter Schottky Institute and Physics Department, TUM School of Natural Sciences, Technical University Munich; [2]Department of Chemistry, TUM School of Natural Sciences, Technical University Munich

P2: ASYMMETRIC ACCEPTOR DESIGN WITH FUSED-IMIDAZOLE LINKAGES FOR EFFICIENT ORGANIC SOLAR CELLS

Liping Liu[1], Enwei Zhu[2], Dirk Guldi[1]
[1]Friedrich Alexander University Erlangen-Nürnberg, Germany; [2]Jilin Normal University, China

P3: BOUND- AND FREE EXCITON EMISSION IN I-III-VI QUANTUM DOTS

Julian Georg Mann, Yizhuo Xi, Bonifasius Auriel Putranto Herard, Leonhard Meurer, Sushant Ghimire, Jochen Feldmann
Chair for Photonics and Optoelectronics, Nano-Institute Munich and Department of Physics, Ludwig-Maximilians-Universität (LMU), Königinstr. 10, 80539 Munich, Germany

P4: CHARGE TRANSPORT AND INTERFACIAL CHARACTERISTICS OF ALD CORROSION PROTECTION LAYERS ON SEMICONDUCTOR LIGHT ABSORBERS

Julius Kühne[1,2], Tim Rieth[1,2], Ian D. Sharp[1,2]
[1]Walter Schottky Institute, Technical University of Munich, Am Coulombwall 4, 85748 Garching, Germany; [2]Physics Department, TUM School of Natural Sciences, Technical University of Munich, Am Coulombwall 4, 85748 Garching, Germany

P5: Dexter Energy Transfer from Quantum Dots to Closely-Bound Dye Molecules

Mariam Kurashvili[1], Jordi Llusar[2], Lena S. Stickel[1], Tim Würthner[1], David Ederle[1], Ivan Infante[2,3], Jochen Feldmann[1], Quinten A. Akkerman[1]
[1]1 Chair for Photonics and Optoelectronics, Nano-Institute Munich, Department of Physics, Ludwig-Maximilians-Universität (LMU), Königinstraße 10, 80539 Munich, Germany; [2]BCMaterials, Basque Center for Materials, Applications, and Nanostructures, UPV/EHU Science Park, Leioa 48940, Spain; [3]Ikerbasque Basque Foundation for Science, Bilbao 48009, Spain

P6: Effects of rotatable groups on metal organic frameworks

Thomas Bergler[1,2], Prof. Dr. Harald Oberhofer[1,2]
[1]Bavarian Center for Battery Technologies (BayBatt), Germany; [2]Chair for Theoretical Physics VII - Computational Materials Design, University of Bayreuth, Germany

P7: Excited state dynamics and performance optimization of diketoprrolopyrrole-based DSSCs for solar energy conversion

Maximilian Herm
Friedrich-Alexander-Universität, Germany

P8: EXTRACTION OF HOT CARRIERS IN COLLOIDAL CSPBBr3 NANOCRYSTALS

Yongqiang Chai[1], Xianjie Chen[2], Dirk Guldi[1]

[1]Friedrich Alexander University Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen, Germany;
[2]Southwest University of Science and Technology, Mianyang, 621010 P. R. China

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P9: First-principles study of phenolic anchor groups for molecular water oxidation catalysts on modified WO₃ surfaces

Matthias Knodt, Emmi Gareis, Stephan Kümmel

Universität Bayreuth, Germany

P15: INFLUENCE OF TEMPERATURE AND LIGHT ON THE STRUCTURE OF LEAD HALIDE PEROVSKITE NANOCRYSTALS

Thomas Baier[1], Huaying Zhong[1], Xiongzhuo Jiang[1], Altantulga Buyan-Arivjikh[1], Andrei Chumakov[2], Sarathlal Koyiloth Vayalil[2], Peter Müller-Buschbaum[1]

[1]TUM School for Natural Sciences, Chair for Functional materials, 85748 Garching, Germany;
[2]Deutsches Elektron-Synchrotron DESY, Notkestraße 85, 22603 Hamburg, Germany

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P11: Guest-Mediated Modulation of Photophysical Pathways in a Coronene Bisimide Cyclophane

Hanna Hoh[1], Jessica Rühe[1], Kavya Vinod[2], Kazutaka Shoyama[1,3], Mahesh Hariharan[2], Frank Würthner[1,3]

[1]Institut für Organische Chemie, Julius-Maximilians-Universität Würzburg, Germany; [2]School of Chemistry, Indian Institute of Science Education and Research Thiruvananthapuram, India; [3]Center for Nanosystems Chemistry, Julius-Maximilians-Universität Würzburg, Germany

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P12: HIGH-PRESSURE METHODOLOGY FOR CLARIFYING PCET MECHANISMS IN GROUND AND EXCITED STATES

Daniel Langford[1], Robin Rohr[2], Stefan Bauroth[1], Achim Zahl[2], Alicja Franke[3], Ivana Ivanovic-Burmazovic[3], Dirk M. Guldi[2]

[1]FAU Erlangen-Nürnberg & ICMM, Erlangen, Germany; [2]FAU Erlangen-Nürnberg, Erlangen, Germany; [3]Ludwig-Maximilians-Universität München, Germany

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P13: Homoleptic Complexes of Bis(4-carboxylpyrazol-1-yl)acetic acid: a New Building Unit for MOFs

Polina Klypina[1], Wintana Tzegai[1], Michaela Reil[1], Markus Fischer[2], Martin Hartmann[2], Nicolai Burzlaff[1]

[1]Department of Chemistry and Pharmacy, Friedrich-Alexander-Universität Erlangen-Nürnberg; [2]Department of Chemical and Biological Engineering (CBI), Friedrich-Alexander-Universität Erlangen-Nürnberg

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P14: Influence of Carbonyl Functionalization in a Molecular Cleft on O-O Bond Formation Mechanism in Light-Driven Water Oxidation

Daniel Friedewald, Olga Anhalt, Frank Würthner

Julius-Maximilians-Universität Würzburg, Germany

P15: Giant rare-earth catecholate crystals- morphology control and rapid NIR luminescence response

Marina Schönherr
LMU, Germany

P16: INTRAMOLECULAR DOWN- AND UP-CONVERSION IN DIMERIC TETRACENE COMPLEXES CENTERED VIA PLATINUM(II) AND PALLADIUM(II)

Yifan Bo[1], Yuxuan Hou[2], Melchor Matabuena[2], Rik R. Tykwinski[2], Dirk M. Guldi[1]
[1]Friedrich-Alexander-Universität Erlangen, Germany; [2]University of Alberta, Canada

P17: Investigating the iodoplumbate complex evolution of perovskite solution during spin coating via UV-VIS in-situ spectroscopy

Maximilian Spies, Simon Biberger, Fabian Eller, Eva M. Herzig, Anna Köhler
University of Bayreuth, Germany

P18: INVESTIGATIONS ON THE OPTOELECTRONIC PROPERTIES OF COMPOUNDS BEARING SMALL HOMOATOMIC CLUSTERS OF THE TETREL ELEMENTS

Dominik Dankert, Yulia Kuznetsova, Sabine Zeitz, Thomas F. Fässler
TUM, Germany

P19: LANGMUIR-BLODGETT PREPARED P-N-JUNCTION POLYMER FILMS AS A PLANAR HETEROJUNCTION IN ORGANIC-BASED SOLAR CELLS

Casmelin R. Nah, Kirill Gubanov, Yana Reva, Maximilian Herm, Dirk M. Guldi, Rainer H. Fink
Department of Chemistry and Pharmacy, Friedrich-Alexander-Universität Erlangen Nürnberg, Egerlandstraße 3, 91058 Erlangen, Germany

P20: Learning an effective hamiltonian of temperature-dependent electronic structure using machine learning

Martin Schwade, Shaoming Zhang, David A. Egger
TUM, Germany

P21: Mechanistic Investigations of the Disulfide Activation Process

Lukas Santiago Diaz
Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

P22: Mechanistic Investigations of the Disulfide Activation Process

Lukas Santiago Diaz
Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

P23: Mapping the photocatalytic reactive sites of 2D materials

Olivier Henrotte[1,2,3], Franz Gröbmeyer[1], Seryio Saris[1,4], Christoph G. Gruber[1], Ismail Bilgin[5], Alexander Högele[5], Naomi J. Halas[3,6], Peter Nordlander[3,6], Emiliano Cortés[1], Alberto Naldoni[7]
[1]Nanoinstitute, LMU, Germany; [2]RCPTM, Palacký University Olomouc, Czech Republic; [3]Technical University of Munich (TUM) Institute for Advanced Study (IAS), Germany; [4]Department of Chemical Engineering, Massachusetts Institute of Technology,USA; [5]Fakultät für Physik, Munich Quantum Center, and Center for NanoScience (CeNS), LMU, Germany;

[6]Department of Chemistry, Department of Physics and Astronomy, Department of Electrical and Computer Engineering, Rice University, USA; [7]Department of Chemistry and NIS Centre, University of Turin, 10125 Turin, Italy

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P24: MULTISTATE PHOTOSWITCHES BASED ON NEARLY PANCHROMATIC NORBORNADIENE-TRIAZINE HYBRID STRUCTURES AS POTENTIAL DATA STORAGE SYSTEMS

Daniel Krappmann, Erik J. Schulze, Harald Maid, Andreas Hirsch
Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

P25: Overcoming Optical Losses in Thin Metal-Based Recombination Layers for Efficient n-i-p Perovskite-Organic Tandem Solar Cells

Jingjing Tian[1,2], Chao Liu[1,3], Larry Lüer[1], Christoph J. Brabec[1,3]
[1]Institute of Materials for Electronics and Energy Technology (i-MEET), Department of Materials Science and Engineering, Friedrich-Alexander-Universität Erlangen-Nürnberg, Martensstraße 7, 91058 Erlangen, Germany; [2]Erlangen Graduate School in Advanced Optical Technologies (SAOT), Paul-Gordan-Straße 6, 91052 Erlangen, Germany; [3]Helmholtz-Institute Erlangen-Nürnberg for Renewable Energy (HI ERN), Immerwahrstraße 2, 91058 Erlangen, Germany

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P26: Plasmonic-induced Thermoelectric Effects in Polymer Electrolytes

Jakob Springer[1], Maximilian Frank[1], Maximilian Rödel[1], Jens Pflaum[1,2]
[1]Experimental Physics VI, University of Würzburg, Germany; [2]Center for Applied Energy Research (CAE), Würzburg, Germany

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P27: PREPARATION AND ISOLATION OF P3HT SUPERSTRUCUTRES WITH DIRECTED ENERGY GRADIENTS

Klaus Kreger
University of Bayreuth, Germany

P28:RANDOM LASING IN FLUORESCENT SILICA AEROGELS: FROM RHODAMINE 6G TO CARBON DOT DOPED COMPOSITES

Anithadevi Sekar, Matthias F Kestler, Theobald Lohmüller, Jochen Feldmann
Ludwig Maximilian University of Munich, Germany

P29: Revealing Degradation Mechanisms in 2D/3D Perovskite Solar Cells under Photothermal Accelerated Aging

Zijian Peng[1,2], Larry Lüer[1], Christoph Brabec[1]
[1]Institute of Materials for Electronics and Energy Technology (i-MEET), Friedrich-Alexander-Universität Erlangen-Nürnberg; [2]Graduate School in Advanced Optical Technologies (SAOT)

P30: Self-Assembly of Nitrogen-Doped Helical Aromatic Bisimides into J-Aggregates

Louis Schramm, Xiaoqi Tian, Vladimir Stepanenko, Matthias Stolte, Frank Würthner
Julius-Maximilians Universität Würzburg, Germany

P31: Structural Analysis of Lead Halide Perovskites

Lukas Max Rescher, Bert Nickel
Ludwig-Maximilians Universität München, Germany

P32: Supramolecular Porphyrin-Perylenebisimide Bola-Amphiphiles

Erik Schulze[1], Elena Mack[1], Christian Ritterhoff[1], Ufuk Borucu[2], Bernd Meyer[1], Dirk Guldi[1], Andreas Hirsch[1]

[1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany; [2]GW4 Facility for High-Resolution Electron Cryo-Microscopy, University of Bristol, Bristol, UK

P33: SYNTHESIS AND CHARACTERIZATION OF CHIRAL ORGANOBORON FOR BIOIMAGE APPLICATIONS

Yuttawat Hashmi

Julius-Maximilians-Universität Würzburg (JMU), Germany

P32: Theoretical determination of tungsten trioxide clusters for photocatalytic water splitting

Emmi Gareis, Matthias Knodt, Stephan Kümmel

University of Bayreuth, Germany

P34: ULTRAFAST DYNAMICS OF A MEROCYANINE DYE-BASED ARTIFICIAL LIGHT-HARVESTING ANTENNA

Rebecca Fröhlich[1], Ajay Jayachandran[1], Alexander Schulz[2], Franziska Schneider[2], Matthias Stolte[3], Frank Würthner[2,3], Tobias Brixner[1,3]

[1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, 97074 Würzburg, Germany; [2]Institut für Organische Chemie, Universität Würzburg, 97074 Würzburg, Germany; [3]Center for Nanosystems Chemistry (CNC), Universität Würzburg, Theodor-Boveri-Weg, 97074 Würzburg, Germany

P35: Unraveling the chirality transfer from circularly polarized light to single plasmonic nanoparticles

Seunghoon Lee[1,2], Chenghao Fan[1], Artur Movsesyan[3], Johannes Bürger[1], Fedja J. Wendisch[1], Leonardo de S. Menezes[1], Stefan A. Maier[1,4], Haoran Ren[4], Tim Liedl[1], Lucas V. Besteiro[3], Alexander O Govorov[3], Emiliano Cortés[1]

[1]LMU München, Germany; [2]Dong-A University, South Korea; [3]Ohio University, United States; [4]Monash University, Australia

P36: Real-space transport channels in halide perovskites

Frederik Vonhoff, Maximilian J. Schilcher, David A. Egger

Technical University of Munich, Germany

Postersession 2 (Sept. 27, 2024 / 10:15 – 11:45)

P1: Advancing photosystem II-based electrodes for photoelectric conversion

Huayang Zhang[1], Philipp Bootz[1], Shaobin Wang[2]
[1]Chair for Photonics and Optoelectronics, Nano-Institute Munich and Physics Department, Ludwig-Maximilians-University (LMU), Munich, D-80539, Germany; [2]School of Chemical Engineering, The University of Adelaide, Adelaide, SA5005, Australia

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P2: Bilayer nanographene with a benzene defect shows evidence for halide permeation

M. A. Niyas
Uni Wuerzburg, Germany

P3: CeTa(O,N)3 and CeNb(O,N)3 perovskite oxynitrides for photoelectrochemical energy conversion

Gabriel Grötzner[1,2], Laura I. Wagner[1,2], Lukas Wolz[1,2], Verena Streibel[1,2], Ian D. Sharp[1,2]
[1]Walter Schottky Institute, TU Munich; [2]TUM School of Natural Sciences

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P4: COVALENT ORGANIC FRAEWORK EMBEDDED WITH SINGLE CU SITES FOR PHOTOCATALYTIC REACTION

Shuo Sun, Jenny Schneider
Ludwig-Maximilians-Universität München, Germany

P5: EFFECT OF CHAIN LENGTH ON THE PHOTOCATALYTIC HYDROGEN EVOLUTION OF POLYMER-TITANIA HYBRID MATERIALS

Teresa Mauerer[1], Julian Hungenberg[2], Mukundan Thelakkat[2], Roland Marschall[1]
[1]Physical Chemistry III, University of Bayreuth, Universitätsstraße 30, 95444 Bayreuth, Germany; [2]Applied Functional Polymers, University of Bayreuth, Universitätsstraße 30, 95444 Bayreuth, Germany

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P6: Enhancing Charge Carrier Transport in Metal (Oxy-)Nitrides for Efficient Solar Fuel Generation

Oliver Brune, Laura I. Wagner, Gabriel Grötzner, Ian D. Sharp, Verena Streibel
Walter Schottky Institut, Technische Universität München, Germany

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P7: EXPLORING PHOTOINDUCED PHASE SEGREGATION IN MAPBI1.5BR1.5 POWDERS

Markus Rainer Griesbach, Fatemeh Haddadi Barzoki, Tobias Siegert, Helen Grüninger, Anna Köhler
University of Bayreuth, Germany

P8: Facet-dependent photovoltaic efficiency and stability variations in mixed Sn-Pb perovskite solar cells

Xiaojing Ci, Xiongzhuo Jiang, Guangjiu Pan, Jinsheng Zhang, Zerui Li, Kun Sun, Peter Müller-Buschbaum
Technische Universität München, Germany

P9: FUNCTIONAL HIERARCHICAL SUPERSTRUCTURES FOR (PHOTO-) CATALYSIS

Dennis Schröder
University of Bayreuth, Germany

P10: GIWAXS STUDIES OF 2D RUDDLESDEN–POPPER PEROVSKITES FOR PHOTOMEMRISTORS APPLICATIONS

Christopher Greve[1], Po-Ting Lai[2], Cheng-Yueh Chen[2], Bo-Yuan Chuang[3], Kai-Hua Kuo[3], Tsung-Kai Su[2], Guang-Hsun Tan[2], Chia-Feng Li[4], Sheng-Wen Huang[4], Kai-Yuan Hsiao[2], Eva M. Herzig[1], Ming-Yen Lu[2], Yu-Ching Huang[4], Ken-Tsung Wong[3], Hao-Wu Lin[2]
[1]Universität Bayreuth, Germany; [2]National Tsing Hua University, Taiwan; [3]National Taiwan University, Taiwan; [4]Ming Chi University of Technology, Taiwan

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P11: Hierarchical electrostatic nanotemplating and self-assembly of electron-transferring hybrid nanostructures for Photocatalysis.

Jyoti Devi, Maximilian Wagner, Franziska Gröhn
Friedrich Alexander university Erlangen-Nuremberg, Germany

P12: Highly Crystalline Oriented (NOP)4AuB3+I8 Gold-based Ruddlesden Popper 2D Double Perovskite thin films as Photodetectors

Florian Wolf[1], Thanh Chau[1], Dan Han[2,3], Patrick Dörflinger[4], Shizhe Wang[1], Rik Hooijer[1], Roman Guntermann[1], Wolfgang Schnick[1], Vladimir Dyakonov[4], Thomas Bein[1]
[1]Department of Chemistry and Center of NanoScience, LMU München, Germany; [2]School of Materials Science and Engineering, Jiling University, China; [3]School of Chemistry, University of Birmingham, United Kingdom; [4]Experimental Physics VI, University of Würzburg, Germany

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P13: Improved Control of Perovskite Thin Film Fabrication via Reactive Spin coating based on Real-Time In-Situ Feedback from Optical Spectroscopy

Simon Biberger, Maximilian Spies, Konstantin Schötz, Frank-Julian Kahle, Nico Leupold, Ralf Moos, Helen Grüninger, Anna Köhler, Fabian Panzer
University of Bayreuth, Germany

P14: INFLUENCE OF SECOND SPHERE MODIFICATIONS ON THE PERFOMANCE OF PORPHYRIN PHOTOCATALYSTS FOR CO2 REDUCTION

Peter Stahl, Christian Wilhelm, Ivana Ivanović-Burmazović
LMU, Germany

P15: Interferometric Scattering in Battery Materials

Franz Gröbmeyer, Mohsen Beladi-Mousavi, Christoph Gruber, Emiliano Cortés
LMU München, Germany

P16: INVESTIGATING GIANT ELECTROSTRICTION IN HALIDE PEROVSKITES WITH DOUBLE MODULATION INTERFEROMETRY

Philipp Ramming
Universität Bayreuth, Germany

P17: Investigation of Binding Motifs in Bioinspired Semisynthetic Zinc Chlorin Aggregates

Michael Bühler, Merle Insa Silja Röhr

University Würzburg, Germany

P18: IRON-DOPED PEROVSKITE CRYSTAL GROWTH FOR ADVANCED OPTOELECTRONIC AND SPINTRONIC APPLICATIONS

Volodymyr Vasylkovskyi[1], Olga Trukhina[1], Anastasiia Kultaeva[1], Patrick Dörflinger[1], Mykola Slipchenko[2], Vladimir Dyakonov[1]

[1]Julius-Maximilians-Universität Würzburg, Germany; [2]Leibniz Universität Hannover, Germany

P19: Lateral π-extended molecular nanographene

Giovanni M. Beneventi[1], Kilian Schöll[1], Fabrizia Negri[2], Alejandro Cadranel[1], Norbert Jux[1], Dirk M. Guldi[1]

[1]Friedrich-Alexander-Universität, Germany; [2]Department of Chemistry "Giacomo Ciamician"

P20: LIGHT-DRIVEN Mn-PORPHYRIN NANOASSEMBLY FOR CATALYSIS

Müge Yücel, Franziska Gröhn

Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

P21: Mechanistic Insights of Tunable Iridium(III) Complexes as Sensitizers for Organic Photocatalysis via Triplet-triplet Energy Transfer

Lukas Alexander Mai

Friedrich-Alexander-Universität Erlangen Nürnberg, Germany

P22: MULTIPLY-FUSED PORPHYRIN-NANOGRAPHENE CONJUGATES

Christoph Oleszak, Christian Lasse Ritterhoff, Max Distel, Bernd Meyer, Norbert Jux

Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

P23: Nanostructure in energy materials

Eva M Herzig

Universität Bayreuth, Germany

P24: PHOTOPHYSICAL PROPERTIES OF CYLINDRICAL MOLECULAR AGGREGATES FOR LIGHT-HARVESTING APPLICATIONS

Lisa Maria Günther[1], Stefan Goppelt[1], Tenzin Kunsel[2], Thomas L. C. Jansen[2], Jasper Knoester[2,3], Jürgen Köhler[1]

[1]Spectroscopy of soft Matter, University of Bayreuth, Germany; [2]Zernike Institute for Advanced Materials, University of Groningen, The Netherlands; [3]Faculty of Science, Leiden University, The Netherlands

P25: Precision excited state calculations in small metal clusters: prototypes for future photocatalytic applications

Nikita Kavka, Simon Herb, Roland Mitric

Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Germany

P26: Production of Thin Films with Inverse Opal Structure via Solluble Alloy Based Precursors

Aimilios Christidis, Christian Fajman, Katja Rodewald, Christian Weindl, Guangjiu Pan, Peter Müller-Buschbaum, Thomas Fässler
TUM School of Natural Sciences, Germany

P27: Vibrational Anharmonicity and Optoelectronic Properties of 2D Perovskites

Chiara Spezzati, Frederik Vonhoff, David Egger
Technical University of Munich (TUM), Germany

P28: Selective Synthesis of Graphene Nanoribbons and the Corresponding Porphyrin Conjugates

Filip Bozinovic, Norbert Jux
Friedrich-Alexander Universität Erlangen-Nürnberg, Germany

P29: Simulating anisotropic photo-physical properties of plexcitons

Luca Nils Philipp
University of Würzburg, Germany

P30: SPUTTER-DEPOSITED TIOX THIN FILM AS A BURIED INTERFACE MODIFICATION LAYER FOR EFFICIENT AND STABLE PEROVSKITE SOLAR CELLS

Xiongzhuo Jiang, Peter Müller-Buschbaum
Technical University of Munich, Germany

P31: SUPPRESSED DEGRADATION PROCESS OF PBDB-TF-T1:BTP-4F-12 SOLAR CELLS WITH SOLID ADDITIVE EH-P

Zerui Li[1], Sergei Vagin[2], Jinsheng Zhang[1], Renjun Guo[1], Kun Sun[1], Xiongzhuo Jiang[1], Tianfu Guan[1], Matthias Schwartzkopf[3], Bernhard Rieger[2], Peter Müller-Buschbaum[1]
[1]Technical University of Munich, TUM School of Natural Sciences, Department of Physics, Chair for Functional Materials, James-Franck-Str. 1, 85748 Garching, Germany; [2]Technical University of Munich, TUM School of Natural Sciences, Department of Chemistry, WACKER Chair of Macromolecular Chemistry, Lichtenbergstrasse 4, 85748 Garching, Germany; [3]Deutsches Elektronen-Synchrotron, Notkestrasse 85, 22607 Hamburg, Germany

P32: Surface Enhanced IR Absorption Spectroscopy to Study the CO2 Reduction Reaction (CO2RR) on Gold Nanostructures

Kai Evan Petersen, Simon Leisibach, Moritz Feil, Katharina Krischer
Technical University of Munich, Germany

P33: Synthesis and Characterization of Expanded Azaborahelicenes

Klaudia Szkodzińska, Agnieszka Nowak-Król
Julius-Maximilians-Universität Würzburg

P34: TOWARDS CD-SPECTROSCOPY OF SINGLE CHLOROSOMES

Stefan Goppelt, Lisa Maria Günther, Jürgen Köhler
University of Bayreuth, Germany

P35: Ultrafast Energy Transfer in Squaraine Oligomers

Laura Lee Haley
Julius-Maximilians-Universität Würzburg, Germany

Notes:

Notes:

Backcover:

SolTech 2024, Nürnberg, 25.-27. Sept. 2024
Conference Schedule

Wednesday, Sept. 25, 2024

Time	Session
12:00-13:00	**Registration & Snacks**
Session 1 / Chair: D. Guldi	
13:00	D. Guldi
13:15	G. Scholes (Princeton)
14:00	L. Kroh (BT)
14:20	S. Krishna (FAU)
14:40	W. Tian (LMU)
15:00 - 15:30	**Coffee Break**
Session 2 / Chair: T. Clark	
15:30	S. Santra (TUM)
15:50	Halkic/Weber (WÜ)
16:10	L. Kumar (BT)
16:30	O. Ferreira (Uberlandia/LMU)
16:50	M. Kestler (LMU)
17:10	F. Negri (Bologna)
18:00	**Session End**

Thursday, Sept. 26, 2024

Time	Session
Session 3 / Chair: NN	
08:30	B. Esser (Ulm)
09:15	W. Kaiser (TUM)
09:35	C. Brabec (FAU)
09:55	K. Sailer (StMWK)
10:05-10:35	**Coffee Break**
Session 4 / Chair: NN	
10:35	Y. Yao (BT)
10:55	J.L. Greenfield (WÜ)
11:15	Le Du (TUM)
11:35	K. Moth-Poulsen (PUC
12:20-13:30	**Lunch Break**
Session 5 / Chair: NN	
13:30	Student Highlights
14:00	L. Elbaz (Bar-Ilan)
14:45	M. Kuhn (BT)
15:10	L. Kreimendahl (WÜ)
15:30 - 16:00	**Coffee Break**
Session 6 / Chair: NN	
16:00	N. Jux (FAU)
16:20	S. Garain (WÜ)
16:40	G. Thomas (IISER, India)
17:30 - 20:00	**Postersession 1 / Hall Ground floor — Poster Session and Get Together**

Friday, Sept. 27, 2024

Time	Session
Session 7 / Chair: NN	
08:30	F. Toma (Hereon, Teltow)
09:15	K. Gubanov (FAU)
09:35	H. Übele (TUM)
09:55	I. Ivanovic (LMU)
10:15 - 11:45	**Postersession 2 / Hall Ground floor — Posters, Coffee & Pastry**
Session 8 / Chair: F. Würthner	
11:45	E. Zysman-Colman (St. Andrews)
12:30	R. Tykwinski (Univ. Alberta)
13:15	N.N.
13:30 -14:30	**Snacks & Goodbye**