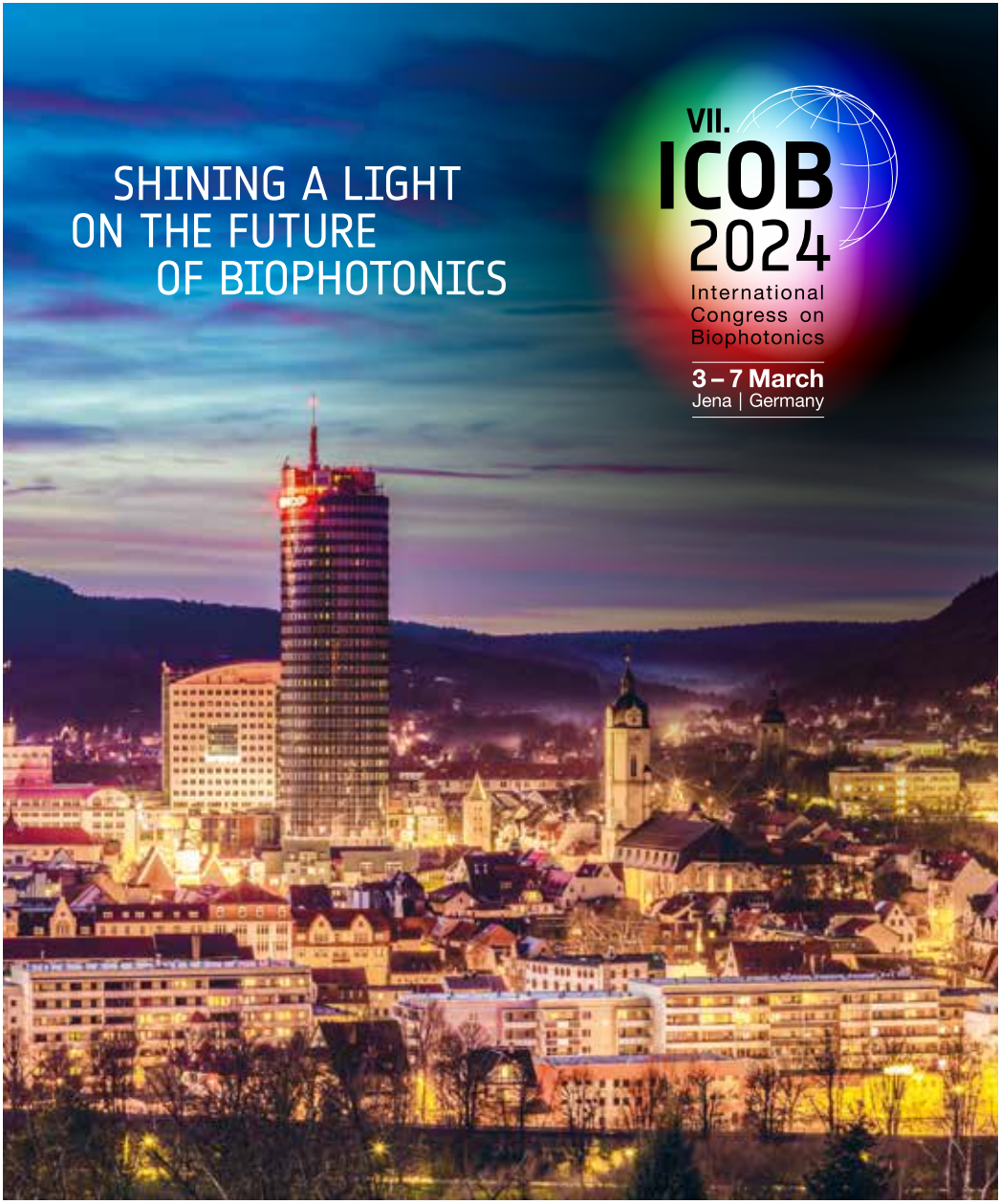

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DGLM Deutsche Gesellschaft für Biophotonik und Lasermedizin e.V.

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DFG Deutsche Forschungsgemeinschaft

FCI Fonds der Chemischen Industrie

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WELCOME TO THE INTERNATIONAL CONGRESS ON BIOPHOTONICS 2024

Juergen Popp
Congress Chair

Dear Participants,

We warmly welcome you to the "City of Light", Jena, and to the 7th International Congress on Biophotonics. This sientific event marks a milestone in biophotonics, uniting researchers, industry experts, medical professionals, and policymakers. This congress focuses on transforming research into market-ready solutions, highlighting the field's potential to revolutionize life sciences.

With around 350 participants, ICOB 2024 is a prime networking opportunity and a hub for the latest developments. ICOB 2024 is organized by the Leibniz Institute of Photonic Technology (Leibniz IPHT) in cooperation with the German Society for Biophotonics and Laser Medicine (DGLM) and presented by Biophotonics4Future. A special highlight is the first-time organization of the X. International Conference on Perspectives in Vibrational Spectroscopy (ICOPVS-2024) in Europe, which enriches and deepens our program.

We also extend our gratitude to the sponsors and supporters of ICOB2024, whose contributions make this event format possible.

Let's shine a light on the future of biophotonics, setting the stage for the next generation of breakthroughs.

Sincerely,
Juergen Popp

WELCOME TO THE CITY OF LIGHT

Let there be light: Jena has embodied competence in this area for over 150 years. As a traditional optics and photonics location, Jena is the cradle of the optical industry in Europe and stands for innovation and progress.

Innovative, light-based technologies have been shaping the science city of Jena for decades. As a European center for research in the field of optics and photonics, the close integration of Jena's two universities with the research institutions and local industry is a tradition and a guarantee of success.

The term “City of Light” is a synonym for everything that made and still makes Jena's supraregional radiance: the flashes of inspiration of its bright minds, the light of enlightenment, the first-class research institutions that constantly bring the light of knowledge into the darkness, the world-famous high-tech companies and the young, innovative people Companies for which light is a key means of success. Light is both a tool and a research object at the same time.

Jena is strong in the life sciences. As anchored in the profile lines “Light Life Liberty” of the Friedrich Schiller University Jena and in the slogan “where life sciences meets physics” of the research campus Beutenberg, interdisciplinary research is carried out.

GENERAL INFORMATION

Date:
3 - 7 March 2024

Venue Address:
Volkshaus Jena // Carl-Zeiss-Platz 15 // 07743 Jena // Germany

Congress Chairmen:

Juergen Popp
Congress Chair

Prof. Wolfgang Kiefer
Honorary Chair of ICOPVS-2024

Congress Organisation:

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Organized by:

Leibniz IPHT

DGLM Deutsche Gesellschaft für Biophotonik und Lasermedizin e.V.

Presented by:

biophotonics 4 FUTURE

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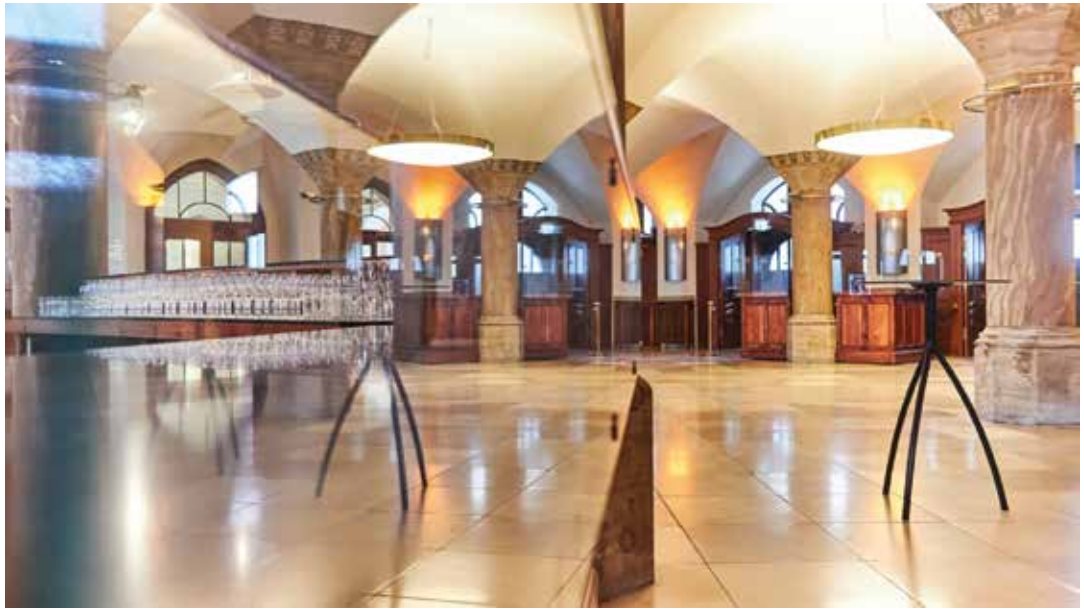


GET-TOGETHER AT VOLKSHAUS JENA
SUNDAY, MARCH 3, 2024

We welcome all participants on the first evening in the reception hall of the conference center. Meet old and new colleagues over snacks and drinks. We wish you a wonderful evening!

You will receive your congress materials at the registration counter.

Venue Address:
Max-Reger-Hall at **Volkshaus Jena**, Carl-Zeiss-Platz 15, 07743 Jena

Time:
start 6 p.m.

CONGRESS DINNER AT VOLKSBAD JENA
TUESDAY, MARCH 5, 2024

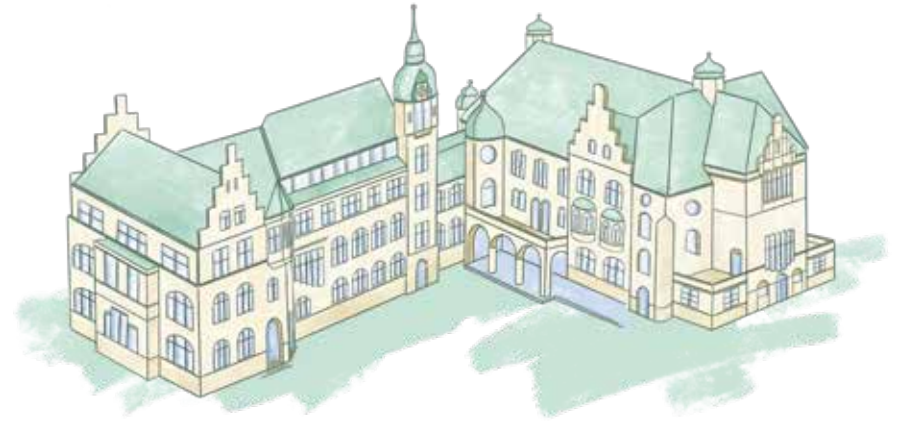
The "Volksbad" in Jena was a public bathing facility that was built between 1907 and 1909 by the Jenaer Volksbad-Verein, officially opened on April 13, 1909. In the early 2000s, it was decided to use the Volksbad as a center for culture and education. It was renovated, with the emphasis on leaving its former use visible. This gives the building a unique charm.
You are cordially invited to spend a social evening together in this special location. Exchange ideas with your colleagues over dinner and drinks.

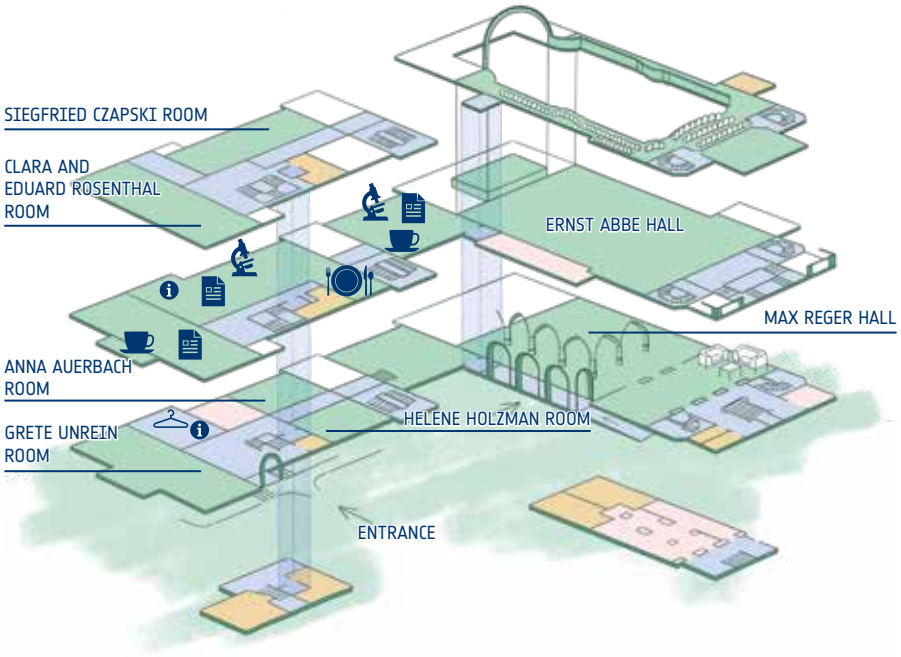
DJ Smoking Joe – one of the best-known DJs from the night scene in Jena and the whole of East Germany will be a great musical accompaniment with his varied repertoire.

Venue Address:
Volksbad Jena Knebelstraße 10 // 07743 Jena // Germany

Time:
start 7 p.m.

VOLKSHAUS JENA





Info/Check-in Catering Coffee Poster Exhibition

PROGRAM OVERVIEW

Sunday, March 3th 2024

6:00 – 9:00 pm

Get-Together & Registration
MAX REGER HALL

Monday, March 4th 2024

9:30 – 10:30 am

Conference Opening &
Keynote by Stefan Hell, Director at the Max Planck Institute for Multidisciplinary Natural Sciences in Göttingen and Nobel Laureate in Chemistry
ERNST ABBE HALL

10:30 – 11:00 am

Coffee Break, Industry Exhibition and Poster Viewing

11:00 am – 12:30 pm

Unmet medical needs: Infections ERNST ABBE HALL	Unmet medical needs: Cancer GRETE UNREIN ROOM

12:30 – 2:00 pm

Lunch Break, Industry Exhibition and Poster Viewing

2:00 – :30 pm

Translation: Challenges ERNST ABBE HALL	Education - B/M, PhD, further Education GRETE UNREIN ROOM

3:30 – 4:00 pm

Coffee Break, Industry Exhibition and Poster Viewing

4:00 – 5:30 pm

Education - Networking, Mentoring, Recruitment
ERNST ABBE HALL

PROGRAM OVERVIEW

Tuesday, March 5th 2024

9:00 – 10:30 am

Applications/ AI-driven Biophotonics – Health: Infections ERNST ABBE HALL	Applications/ AI-driven Biophotonics – Health: Advanced understanding of cell processes and organ functions GRETE UNREIN ROOM	Applications/ AI-driven Biophotonics – Health: Cardiovascular Diseases CLARA AND EDUARD ROSENTHAL ROOM	ICOPVS Short Talks I HELENE HOLZMAN ROOM	ICOPVS Short Talks II ANNA AUERBACH ROOM

10:30 – 11:00 am

Coffee Break, Industry Exhibition and Poster Viewing

11:00 am – 12:30 pm

Applications/ AI-driven Biophotonics – Health: Wellbeing ERNST ABBE HALL	Applications/ AI-driven Biophotonics – Health: Further Topics GRETE UNREIN ROOM	Applications/ AI-driven Biophotonics – Health: Neuro-Degenartive Diseases CLARA AND EDUARD ROSENTHAL ROOM	ICOPVS Short Talks III HELENE HOLZMAN ROOM	ICOPVS Short Talks IV ANNA AUERBACH ROOM

12:30 – 2:00 pm

Lunch Break, Industry Exhibition and Poster Session

2:00 – 3:30 pm

Venturing Beyond the Lab: Translational Research and Venture Capital in Life Sciences ERNST ABBE HALL	Ecosystem – From Research to Markets GRETE UNREIN ROOM	Setting the stage: Linear and nonlinear relationships in IR- and Raman-spectroscopy CLARA AND EDUARD ROSENTHAL ROOM

3:30 – 4:00 pm

Coffee Break, Industry Exhibition and Poster Viewing

4:00 – 5:30 pm

Translation – Best Practice Examples ERNST ABBE HALL	A Potpourri of different AI techniques applied to IR- and Raman-spectroscopy CLARA AND EDUARD ROSENTHAL ROOM

7:00 – 11:00 pm

Congress Dinner
VOLKSBAD JENA, KNEBELSTRASSE 10, 07743 JENA

PROGRAM OVERVIEW

Wednesday, March 6th 2024

9:00 – 10:30 am

Applications/AI-driven Biophotonics – Health: Prevention & Early Diagnosis ERNST ABBE HALL	Applications/AI-driven Biophotonics – Health: Cancer Therapy (Robotics) GRETE UNREIN ROOM	Applications/AI-driven Biophotonics – Health: Continuous Monitoring CLARA AND EDUARD ROSENTHAL ROOM	Applications of AI-assisted vibrational spectroscopy - Chemistry and Materials Science SIEGFRIED CZAPSKI ROOM

10:30 – 11:00 am

Coffee Break, Industry Exhibition and Poster Viewing

11:00 am – 12:30 pm

Industry Session ERNST ABBE HALL	Applications of AI-assisted vibrational spectroscopy – Biology and Medicine SIEGFRIED CZAPSKI ROOM

12:30 – 2:00 pm

Lunch Break, Industry Exhibition and Poster Session

2:00 – 3:30 pm

Applications/AI-driven Biophotonics – Agriculture/Food ERNST ABBE HALL	Applications/AI-driven Biophotonics – Health: Optical Diagnostics GRETE UNREIN ROOM	Applications of AI-assisted vibrational spectroscopy – Process Analytical Technology, Forensic SIEGFRIED CZAPSKI ROOM

3:30 – 4:00 pm

Coffee Break, Industry Exhibition and Poster Viewing

4:00 – 5:30 pm

Applications/AI-driven Biophotonics – Environmental Monitoring ERNST ABBE HALL	Applications/AI-driven Biophotonics – Health: Cancer Therapy (PDT & Surgery) GRETE UNREIN ROOM	Applications of AI-assisted vibrational spectroscopy – Agriculture, Food, Environmental monitoring SIEGFRIED CZAPSKI ROOM

Thursday, March 7th 2024

9:00 am – 2:00 pm

Lab Tour
LEIBNIZ IPHT, ALBERT-EINSTEIN-STR. 9, 07745 JENA

THANKS TO OUR SPONSORS

UNMET MEDICAL NEED – INFECTIONS

4 March // 11 a.m. - 12:30 p.m. // Ernst Abbe Hall
Chair: Michael Bauer

Operation "wharp speed" - How "slow" is contemporary routine diagnostic really?

Bettina Löffler - University Hospital Jena, Institute of Medical Microbiology, Jena, Germany

Diagnostic methods have been largely improved in Medical Microbiology mainly by automatization, better culture methods, and molecular biology techniques (PCR methods and sequencing). Yet, many methods are still work-intensive, expensive, and require incubation steps that take hours/days until the results are reported. Optical methods have the advantage that (i) they are cheap and do not require expensive chemical compounds; so that a high number of samples can be processed. (ii) Optical methods can be designed to be label-free to avoid labor-intensive working steps. (iii) Additionally, host factors could be measured to obtain more information on the infection course.

In my presentation, I will highlight three unmet diagnostic needs in Medical Microbiology, in which optical methods could speed up and improve diagnostics:

- Bacterial infection can be detected by culture methods and the identification of the bacteria is performed by VITEK or MALDI-TOF. Nevertheless, the testing of antimicrobial resistance is still time-intensive, as it requires the growth of the bacteria against different antimicrobial compounds. This is of particular interest in positive blood cultures. Consequently, rapid and easy-to-handle resistance testing is a high medical need. The resistance testing is crucial for the attending physician, who needs to start adequate therapy early to improve the survival of critically ill patients. Optical methods could be used to detect the phenotypic resistance profile of the growing bacteria.
- Many patients are pre-treated with antibiotics when they are admitted to hospital. By culture methods pretreated bacteria often fail to grow and cannot be detected. Even though molecular methods have improved, we do not have a reliable way to detect pretreated bacteria. To improve diagnostics we require reliable methods to detect the presence of microorganisms (including slow-growing and non-culturable pathogens). For this, optical methods could include altered host factors.
- In outbreak or pandemic situations, we experienced a high need for rapid and cheap, but reliable and high sensitive methods to detect a defined pathogen. This is essential to take the right hygiene measures. Optical methods could help to rapidly perform diagnostics without high costs.

Optical methods could provide techniques for the development of novel methods to speed up and improve diagnostics.

Klebsiella, Pseudomonas, Stenotrophomonas ... who cares?"

Mervyn Singer - University College London, London, UK

Infection can trigger sepsis, a life-threatening host response that leads to organ dysfunction. Sepsis is a significant worldwide problem with millions each year dying from this condition. In developed countries mortality is approximately 30% and even in those who survive there is significant short- and long-term morbidity. Bacterial infection, most often due to Gram negative organisms, is the commonest type of infection that leads to sepsis. The mainstay of patient treatment is early and effective source control (e.g. surgery to repair a perforated bowel) and antibiotic coverage. With the rapid progression of antimicrobial resistance, Gram negative organisms in particular are increasingly difficult to treat. The clinician is thus faced with the dilemma as to what antibiotic regimen should be selected that will be effective against the infecting pathogen in that individual patient, and will reach the site of infection in adequate concentration. Knowing the precise genus (Klebsiella, Pseudomonas, etc) is academically interesting and useful for epidemiology purposes. However, from the clinician (and patient) perspective, it is far more useful to identify the right antibiotic(s) to select against which the pathogen will be susceptible. And this need is urgent – delays greater than 6 hours in giving the right antibiotic is associated with worse patient outcomes. This window may be even shorter in the most critically ill patients. The second priority is to give the right dose of antibiotic – too low a concentration increases the risk of suboptimal killing of the pathogen while excessive dosing leads to risks of considerable harm through adverse effects on the immune system, mitochondria, microbiota and organ function. Unfortunately, drug

handling is highly variable in critically ill patients so many patients receiving an equivalent dose achieve blood concentrations that are either too low or too high.

Point-of-care = point-of-need ... what's possible on the ICU?

Michael Bauer - University Hospital Jena, Jena, Germany

UNMET MEDICAL NEED – CANCER

4 March // 11 a.m. - 12:30 p.m. // Grete Unrein Room
Chair: Orlando Guntinas-Lichius

Novel approaches and developments in fluorescence-guided resections of head & neck tumours

Christian Betz - UKE, Hamburg, Germany

Survival of patients with head and neck squamous cell carcinoma (HNSCC) is still insufficient despite state-of-the-art multimodal treatment. A central challenge of surgical treatment particularly in recurrent HNSCC is the complete tumor resection with adequate tumor-free margins based solely on visual and tactile information. Fluorescence-guided surgery represents a promising technique to optimize intraoperative identification of HNSCC margins.
In recent years, various fluorescence-guided surgical concepts have been developed and widely tested in a whole range of clinical conditions. Due to their easy accessibility, tumors of the upper aerodigestive tract have been amongst the those most tested in Phase 2 trials. The probes used ranged from fluorescence-labeled tumor-specific antibodies over nanoparticles / small molecules targeting tumor-specific molecules to pH-activable fluorescent molecules, and lead to remarkable and promising results.
So far, however, none of these molecules have been granted approval for routine clinical use. The most important problems encountered on the road towards clinical approval seem to be difficulties in achieving a high degree of objectiveness or reproducibility, respectively, for example due to inconsistent lighting conditions and camera setups, or due to varying amounts of dye used.
The lecture will introduce the audience to the topic and focus on those points mentioned above. It will provide the participant with a deeper understanding of current developments with regards to novel approaches and developments in fluorescence-guided resections of head & neck tumors.

Narrow Band Imaging (NBI) and Artificial Intelligence (AI) for an Objective Assessment of Upper Aerodigestive Tract Lesions

Christoph Arens - University Hospital Giessen und Marburg, Gießen, Germany

The integration of Narrow Band Imaging (NBI) and artificial intelligence (AI)holds immense promise in revolutionizing the assessment of upper aerodigestive tract (UADT) lesions. NBI is an advanced endoscopic technique that enhances visualization of mucosal structures in the UADT. It utilizes narrow bandwidths of light (415 nm and 540 nm) to highlight vascular patterns and mucosal irregularities. By emphasizing specific wavelengths, NBI improves the detection of subtle lesions, such as early-stage cancers and precancerous changes. The resulting images provide detailed information about the microvascular architecture and surface morphology. AI algorithms, particularly deep learning models, play a crucial role in automating lesion analysis. Convolutional neural networks (CNNs) are commonly employed for feature extraction and classification.

Different studies dealing with NBI and AI are presented. AI systems trained on large datasets learn to recognize patterns indicative of malignancy or dysplasia. Real-time AI analysis assists clinicians in making objective decisions during endoscopy. NBI combined with AI offers several clinical benefits:

- Lesion Detection: AI algorithms identify suspicious areas, aiding in targeted biopsies.
- Classification: AI distinguishes between benign, premalignant, and malignant lesions.
- Margin Assessment: AI helps assess surgical margins during resection procedures.
- Follow-up Monitoring: AI facilitates tracking lesion changes over time.

Integration of NBI and AI reduces interobserver variability and enhances diagnostic accuracy. Challenges include standardization, validation, and seamless integration into clinical workflows. In summary, the synergy between NBI and AI represents a paradigm shift in UADT lesion evaluation, empowering clinicians with precise, data-driven insights for improved patient care.

References:

1. Esmaeili N, et al., Sci Data. 2023 Oct 21;10(1):733. doi: 10.1038/s41597-023-02629-7.
2. Esmaeili N, et al., Sensors (Basel). 2021 Dec 6;21(23):8157. doi: 10.3390/s21238157.
3. Esmaeili N, et al., Diagnostics (Basel). 2021 Mar 3;11(3):432. doi: 10.3390/diagnostics11030432.

Multimodal imaging for delineation of resection marginsduring cancer surgery

Orlando Guntinas-Lichius, Orlando - Jena University Hospital Jena, Germany

Complete tumor removal with tumor-negative resection margins play a crucial role cancer surgery is essential for reduced risk of tumor recurrence and improved survival of the patient. State-of-the-art for intraoperative definition of the tumor margins is based on white light inspection, endoscopy or microscopy of the tumor, and the surgeon's experience. This can be imprecise and leads to incomplete tumor resection, higher risk of recurrence and worse survival. Biophotonic techniques for an intraoperative tumor assessment in combination with an artificial intelligence based online evaluation of the tumor surface are urgently needed to allow a better guidance of the tumor resection to reach a higher probability of a complete tumor removal but sparing functionally important normal surrounding tissue.

The lecture will give an overview of the research of an interdisciplinary working group from Jena including chemists and physicists from the Leibniz Institute of Photonic Technology (Leibniz IPHT), computer scientists from the Friedrich-Schiller-University, engineers form the University Ilmenau, partly in cooperation with European partners.

Main focus is microscopy and endoscopy based marker-free multimodal non-linear imaging and Raman imaging. Both techniques allow already now ex vivo on tissue slides a very reliable distinction between tumor tissue and neighboring normal tissue. At the moment, the transfer to an intraoperative frozen section scenario, and the analysis of bulky unprocessed tissue is realized. As a very important step, the first in vivo clinical trial to show the feasibility of Raman spectroscopy for intraoperative diagnostics during head and neck cancer surgery was started in 2023.

Open questions are optimal visualization for intuitive intraoperative guidance of the oncosurgeon, implementation into robotic devices, and the establishment of a network for multicenter trials.

Funded by Carl-Zeiss-Foundation (program: CSZ breakthroughs), Federal Ministry of Education and Research (BMBF: Theraoptik 13GW0370E), Horizon 2020 (101016923 [CRIMSON]), and Horizon Europe program (101058004 [CHARM]).

TRANSLATION – CHALLENGES

4 March // 2 - 3:30 p.m. // Ernst-Abbe Hall
Chair: Jens Hellwage

Wastewater-based epidemiology – opportunities and hurdles

Robert Möller - Analytik Jena GmbH+Co.KG, Jena, Germany

During the corona pandemic wastewater-based epidemiology was a prominent topic. Different approaches were developed to detect fragments of the virus in wastewater samples. The information from the wastewater could serve as an additional source of information for assessing the situation. Even so many advances have been made in the last years wastewater-based epidemiology is not yet a widely used tool.
The talk will describe the development of a practical workflow for the analysis of wastewater samples and describe further advances in the sampling process and automation of the analysis. The workflow is suited for the monitoring of a wide variety of pathogens and can easily implemented a various test site. Furthermore, the talk will focus on the challenges that need to be addressed in order the make wastewater-based epidemiology a reliable tool.

Non-Invasive Blood Glucose Measurement: From the Idea to a Medical Device

Werner Mäntele - DiaMonTech AG, Berlin, Germany

Worldwide, more than 500 Million people live with diabetes. Diabetes cannot be cured, but managed by strict control of blood glucose and adaptation of food intake, physical activity and medication. Blood glucose control presently involves finger pricking and analysis of a drop of blood by a test strip – a painful and uncomfortable procedure. Consequently, many research groups, startups and companies worldwide search for the „holy grail“ of non-invasive and painless blood glucose measurement.

In the talk, the tedious steps from the initial idea of an infrared-based technology in our research group at Frankfurt University to the proof of principle and the proof of concept (TRL 1- TRL 3) and the validation of the technology in the laboratory (TRL 4) are described. The important role of protection of IP in that early phase is discussed. Since most universities cannot provide a beneficial and cooperative environment for further steps and potential industry partners considered the development project as „ very interesting and promising, but too early“, foundation of a startup „DiaMonTech“ (for Diabetes Monitoring Technology) seemed the adequate step to overcome the „valley of death“ in translation. This will be described along with the different funding campaigns and installation of SOPs for the further development. In the company and with contributions from external partners, technology could be further developed to a table-top prototype that serves as a technology carrier and for clinical studies (TRL 5 – TRL 7).
The validation of the technology in clinical settings and the compliance with the guidelines for medical products (e.g. CE approval) as well as DIN and ISO certifications are time-consuming and labour-intensive steps but are clearly outside the scope for university groups. Finally, a prototype of a handheld, IR-Laser-based device can be presented (TRL 8) that will be ready for production in 2025.

From project to company: Strategic challenges for startups

Klaus Schindlbeck - Aspirion Consult, Tuttlingen, Germany

EDUCATION - BACHELOR/MASTER, PHD, FURTHER EDUCATION

4 March // 14 - 15:30 p.m. // Grete Unrein Room
Chair: Heidi Ottevaere

An Integrated MSc Program: Theory, Practical Experience and Industry Insight in Biophotonics

Heidi Ottevaere - Vrije Universiteit Brussel, Brussels, Belgium

Biophotonics, a multidisciplinary field at the intersection of biology, photonics and optics, plays a pivotal role in advancing medical diagnostics, imaging, and therapeutic interventions. This abstract presents an innovative and comprehensive training program designed for Master of Science (MSc) students, emphasizing a balanced integration of theoretical knowledge, hands-on practical courses, and industry visits in biophotonics.

The theoretical component of the program delves into fundamental principles of optics, photonics, and their applications in the life sciences. The curriculum spans topics such as light-matter interactions, imaging techniques, spectroscopy, and the latest advancements in biophotonics technologies and machine learning. This theoretical foundation provides students with a robust understanding of the underlying principles governing the field.

Complementing the theoretical aspects, the program places a strong emphasis on hands-on courses to cultivate practical skills. Students engage in laboratory sessions where they apply theoretical concepts to design and conduct experiments using state-of-the-art biophotonics instrumentation. These hands-on experiences not only reinforce theoretical learning but also foster critical thinking, problem-solving, and experimental design skills essential for future research and development in biophotonics.

To bridge the gap between academic knowledge and real-world applications, the program incorporates company visits and industrial networking events as a vital component. Students can interact with professionals in the biophotonics industry, gaining insights into the practical challenges and innovations shaping the field. These visits provide a valuable context for students to understand how theoretical concepts are translated into commercial products and applications, preparing them for careers in both academia and industry.

In conclusion, the MSc program outlined in this abstract offers a holistic approach that equips students with a deep theoretical understanding, hands-on technical skills and industry awareness. This multifaceted training strategy aims to produce well-rounded professionals capable of contributing meaningfully to the dynamic and rapidly evolving field of biophotonics.

International Graduate summer school Biophotonics

Peter E. Andersen - Technical University of Denmark, Kongens Lyngby, Denmark

Exploring Biphotonic through Game-Based Learning

Fabio Chiarello - Institute for Photonics and Nanotechnologies (IFN-CNR), Rome, Italy

This presentation showcases innovative approaches to science education and dissemination in biophotonics, highlighting experiences conducted at IFN-CNR. The focus lies in employing game-based methodologies for engaging different audiences, including students, educators and the general public.

Some examples of board games developed to introduce participants in different thematic will be presented. For example, “Quantum Race”, on the principles of Quantum Mechanics, or “LigtHiT”, where the refraction of a laser beam must be used to hit targets. Some of these board games have been proposed in live adaptations on an oversized scale, immersing participants as players, for example in "Lab-on-Chip", at exploration of nanobiotechnologies.

In further experiences, participants have been involved in the process of designing scientific board games, for example during creative laboratories. In particular it will be presented "Fotonica in Gioco" ("Photonics at Play"), a competition engaging high school students in the development of educational board games based on predefined themes, organized in Italy by IFN-CNR since 2015.

These experiences, obtained results and future perspectives will be presented and discussed.

Spread Biophotonics: from the university to the citizens

Rebecca Re - Politecnico di Milano, Milano, Italy

At the department of physics of Politecnico di Milano, a quarter of the employee (professors, researchers, Post-PhD and PhD), works in the field of biophotonics developing innovative techniques mainly aimed at non-invasive diagnostic applications.
The Third Mission of the Italian university supports the two main functions of the university, scientific research and training, with the precise mandate of spreading culture, knowledge and transferring the results of research outside the academic context, contributing to the social growth and cultural direction of the territory.
These two components, combined together, makes our department very active in organizing a high number of initiatives of different nature, for spreading biophotonics at various categories of final user. The objectives of these actions span from teaching at high level of education to the dissemination for bringing ordinary people closer to this sector, which it is often considered as aimed at only a niche group of users or too difficult to be understood.
During the presentation, a wide range of examples will be illustrated, starting from educational events in primary and high schools, where the principal teaching tools are experiences and experiments. We will then move on to very specialized university courses, for the Bachelor and master degree up to the PhD program.
Projects specifically designed to drive the alumni, after their university studies, towards the corporate world will be presented and in turn bring companies operating in the biophotonics sector closer to the university environment. Examples of successful start-up will be also given.
Student associations in the biophotonics sector will be shown together with their joint action for the dissemination of this field among citizens, therefore a non-specialized target.
Finally, an overview on specific projects that encourage the circulation of researchers in the field of biophotonics will be given.
With this 360-degree approach to the biophotonics teaching and spreading, it will be interesting to understand how the methodologies, language and register change in different contexts, as does the objective of the action considered.

EDUCATION - NETWORKING, MENTORING, RECRUITMENT

4 March // 4 - 5:30 p.m. // Ernst Abbe Hall
Chair: Katarina Svanberg

Being carried across three continents by the optics community

Inga Saknīte - University of Latvia, Riga, Latvia

Driven by curiosity and willingness to improve patient care through light-based technologies, I have been fortunate to connect and work with dedicated researchers from around the world. I will share my experience on how networking has helped me find and recognize exceptional mentors. All of us, especially in the early stages of our careers, need and deserve a great mentor who inspires and supports us in recognizing our skills and talents and helps us achieve our full potential.
I am a Leading Researcher at the Biophotonics Laboratory, the University of Latvia, and an Adjoint Assistant Professor in Dermatology at the Vanderbilt University Medical Center in Nashville, Tennessee, the United States. My main research interest is advancing noninvasive imaging technologies to quantitatively assess skin for clinical impact. Among other projects, I am currently leading photodocumentation of patients with mpox as part of a randomized controlled trial in the Democratic Republic of the Congo. I have multiple years of research experience in photographic, hyperspectral, and microscopic imaging of human skin, standardized protocol and guideline development, image processing and analysis, and device and algorithm development.
I received PhD in physics from the University of Latvia in 2016. I was then awarded the Fulbright Scholarship to advance my translational research career at the Beckman Laser Institute of the University of California, Irvine. From 2017 until 2021, I was a Postdoctoral Research Fellow at the Vanderbilt Dermatology Translational Research Clinic (VDTRC.org), and was named the inaugural Vanderbilt Postdoctoral Mentor of the Year in 2021.

Clinical work and research activity – a problematic equation

Katarina Svanberg - Lund University, Lund, Sweden

Biophotonics is a field that has developed immensely during the last 20 years. When first started it included a few groups worldwide with giant scientists like Britton Chance and others. Soon the learned societies, e.g., SPIE, OPTICA (former OSA) and IEEE, initiated conferences in the field. The SPIE conference Photonics West very quickly included Biophotonics as a substantial part of the program. An effort started with jointly organized conferences in Europe held in connection with the large exhibition in Munich.

One important aim stated by the learned societies was to build up platforms for networking, serving scientists from various disciplines, to facilitate interdisciplinary discussions concerning possible clinical problems. The driving force in the interaction between the medical doctors and the technical people should be a medical "pull" from the health care sector rather than a technical "push". The aim to build up interdisciplinary platforms is certainly adequate, but the problem was and still is that the situation for clinically active medical doctors does not allow too much time for such activities. This situation has not been developing in the "right" direction, rather the opposite. It is certainly difficult to reach a percentage of 10 for clinical doctors at the Biophotonics conferences. With heavy workload and shrinking economical resources within the health sector, the situation is somewhat critical. These aspects are more general. In many cases the medical doctors, in particular the young one, have to "buy free" time for research. This of course differs from region to region and from country to country but in general this is true.

Translational research within Biophotonics has, even in the situation described, been able to develop and transfer some real successful techniques in the twilight zone between physics and medicine and has led to dramatic improvement in the handling of patients. This really shows the strength, devotion, persistence and skill among active physicists working together with highly motivated research-interested medical doctors. One such example is Optical Coherence Tomography (OCT), which has revolutionized the sector of ophthalmology. Every patient these days coming to the ophthalmologist¨s office for retinal investigation has an OCT diagnostic procedure performed. Another important contribution to the medical "tool box" is the Raman spectroscopy-based bacterial classification in relation to adequate antibiotics to be chosen in the serious event of an upcoming sepsis. The oncology sector, and particularly oncological dermatology, has also been offered an efficient treatment modality with very few side effects, namely Photodynamic Therapy (PDT). This modality offers the patient with non-melanoma malignant skin tumors a perfect therapy with excellent efficacy and almost no cosmetic signs. The follow-up development of PDT with interstitial approach makes it possible to reach also deep lying tumors in the body. This applies, e.g., for prostate cancer, the number one cancer type for men, which recently over-numbered male lung cancer. A critical decision for these patients is if there should be a treatment or not, taking into account the natural history of the disease, and the induction of unwanted side effects. However, with fiber-based focal therapy with detailed and interactive laser light dosimetry, the tumor could be eradicated with minimal side effects. This is still to be proven but ongoing clinical trials will certainly give indications and open a completely new way of handling this increasing number of patients worldwide.

Interdisciplinary approaches and collaboration with the commercial sector are key issues for open up for new ways of ruling the health sector with an aging population and shrinking economical resources.

Pursuing and promoting science – a multi-faceted endeavor

Sune Svanberg, Department of Physics, Lund University, Lund, Sweden

Based on over 50 years of experience in pursuing and promoting science, including 40 years in biophotonics, the author will share some personal thoughts on "how to do things".

The topic is certainly complex and moving forward is an iterative process, where a lot of learning from mistakes certainly has its place. Like in fostering children, giving advice to young people in science is mostly a question of "sending them off in the right direction", and coping with issues as they appear. The most important thing about getting anywhere in science is to create enthusiasm, and to be driven by a quest for new understanding, and to contribute to the world becoming a better living place for all. Here the role of teaching and thesis advisor-ship is paramount – and here you find the greatest multiplication effect on your efforts – potentially helping young people to become more successful than yourself being an ultimate goal to strive for. Also, giving students from less favored regions the pos-

sibilities to contribute to the development of their own societies is a particularly rewarding activity.

A good working atmosphere in a research group – where all are appreciated and included - is a basis for successful science. Talent must be allowed to grow – it should then be remembered, that "in the shadow of big trees little or nothing is growing". Science is mostly an endeavor of interaction and collaboration – structures for facilitating these aspects can be networks and center formations. Some experience from Lund University will be shared, taking the Lund Laser Centre (LLC) and the Lund University Medical Laser Centre (LUMLAC) as examples. Mentoring is an important ingredient, which can be very helpful at all levels in an academic career. Experience from guiding a Swedish group of selected "Research Leaders of the Future" will be shared.

Interdisciplinary approaches and openness to innovation and unconventional thinking are key ingredients to most areas of basic as well as applied research. Patent writing and industrial collaboration are also necessary tools to ensure that scientific progress can have a fast impact on society.

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APPLICATIONS/AI-DRIVEN BIOPHOTONICS – HEALTH: INFECTIONS

5 March // 9 - 10:30 a.m. // Ernst-Abbe Hall

Chair: Jürgen Popp

Raman-based assays to characterize the cellular immune response: from in-vitro assays towards clinical trials

Ute Neugebauer, Leibniz Institute of Photonic Technology, University Hospital Jena, Jena, Germany

Raman spectroscopy is a powerful biophotonic technology that can deliver in-depth information about biological specimen in short analysis time in a labelling-free and non-destructive manner. Recent technological advances made it possible to collect spectral information from individual cells in high-throughput, paving the way for potential diagnostic applications. Immune cells, crucial components of the immune system, help to defend the body against invading pathogens and foreign substances. Understanding and monitoring the cellular immune response can provide valuable insights into the body's defense against pathogens, but also to assess the impact of immunotherapeutic interventions, to just name a few. Circulating immune cells from peripheral blood can be easily obtained from minimal amounts of blood. With appropriate tools that allow monitoring individual immune responses, tailoring treatments based on a patient's specific immune profile could lead to a personalized precision medicine that leads to increasing the likelihood of successful outcomes for specific patients. This contribution will present how Raman spectroscopy is used to characterize immune cells, differentiate their phenotype, and follow their response to pathogens and pathogen-associated molecular patterns (PAMPS). We will start with results obtained in the controlled environment of in vitro assays and discuss how Raman spectroscopic fingerprints of THP-1 monocytes after stimulation can be correlated to the activation state of the cells providing valuable insights into the cellular immune responses. In a similar manner could the Raman spectroscopic signature be used to differentiate the cause of infection of primary isolated human leukocytes after in-vitro stimulation with intact bacterial and fungal pathogens. Ultimately, the aim is to translate these powerful biophotonic techniques also to the bed side to use the promise of rapid, sensitive, and specific Raman-based assessments of immune status in patients. For this, sample preparation and collection devices have been optimized. In a first translational trial, the added value of the Raman spectroscopic leukocyte profile was demonstrated for the identification of infection and sepsis.

Acknowledgements:

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Trends and opportunities in light-based infection diagnosis

Anja Silge, Leibniz Institute of Photonic Technology, Jena, Germany

Cellular signatures captured by laser light and analyzed by vibrational spectroscopy methods such as IR and Raman spectroscopy have shown enormous potential in investigating the host response to infections, bacterial pathogen characterization, and medical diagnostics. Increased interdisciplinary dialogue between spectroscopists and end users, such as clinicians, defines analysis scenarios that steer instrumental developments and system integrations towards small, compact devices and intelligent workflows with integrated sample processing, thus generating new potentials for pathogen and infection diagnostics.
Finding a common language between technologists and physicians leads to mutual understanding, which is essential to successfully and efficiently querying the attributes of a sample. On the one hand, it is about distinguishing between diseased and healthy cells or sensitive and resistant bacteria in a sample. On the other hand, it is critical to understand how these states must be sampled and evaluated using photonic methods in order to exploit the method's potential, namely non-destructive and label-free sampling of sample-inherent features. The task of us technologists is to make the method so robust, reliable and comprehensible that the correct diagnostic conclusions can be drawn from the measurement results. The development of clinical workflows and tailored sample preparation procedures that automatically handle small sample volumes in appropriate sample collecting units opens up new fields of study and innovation. Measurement standardization through appropriate test and reference methods, data management, and evaluation strategies that place physical measurement data in a diagnostic context. The lecture provides an overview of emerging trends and opportunities in light-based infection diagnosis.

Xplore the Digital Dimension

Theresa Liebe - BLINK AG, Jena, Germany

Blink develops an open platform – the BLINK beads.
We are a growing company based in Jena that develops rapid, sensitive and quantitative multiplex assays. Our first application is a rapid multiplexing digital PCR for the point of need. Our technological approach is focused on combining all critical steps of an analytical workflow in a single, undisrupted sample-to-answer workflow. The key to this is a novel reagent which we call the BLINK nanoreactor beads. The surface enables the extraction of nucleic acid from a variety of different sample types and the inner space enables extensive multiplex target amplification. The nanoreactor beads have the ability to quantitate each individual target and if necessary to test for the specificity of the amplification reaction. Multiplex applications are implemented with fluorescent labels, which serve as an address for target specific primers and probes that can be attached individually to our beads. During the analysis process primers and probes are released and the space formed by the hydrogel serves as a discrete amplification compartment. Our encoding is based on detecting the presence or absence of a fluorescent label. This binary approach makes label identification robust and specific. In order to provide a tool for exploring and developing assays based on nanoreactor beads, we developed a new product, the BlinkX. If you are interested in the technology, please join the presentation or reach out to me or my colleagues.

From Bench to Bedside - Approval and Reimbursement of Diagnostic Tests in Germany and Europe

Anni Matthes - Friedrich Schiller University, University Hospital Jena and InfectoGnostics Research Campus, Jena, Germany

Robby Markwart - Friedrich Schiller University, University Hospital Jena, Jena, Germany

With an increasing emphasis on ensuring the safety and efficacy of medical devices, the CE certification process has become a pivotal gateway for market access in the European Union (EU). The In vitro Diagnostic Medical Devices Regulation (IVDR) shapes the CE certification process on EU level, which is harmonized across all EU members. Simultaneously, reimbursement policies play a critical role in determining the economic viability and widespread adoption of diagnostic tests. The IVDR sets the framework for CE certification within EU members, while reimbursement policies diverge among member states.
In this presentation, we give a brief overview of the European CE certification process with focus on photonics-based diagnostics, including risk classification, conformity assessment, required clinical evidence and post-market surveillance. Furthermore, we will discuss different healthcare and reimbursement systems in Europe from the perspective of diagnostic test developers and manufactures. Both, CE certification and reimbursement may require evidence on the clinical safety, efficacy and effectiveness. Therefore, we will summarize different types of clinical evidence and corresponding study designs, to support studies that yield evidence that is relevant for official authorities. Finally, we provide an outlook on the requirements for translating a diagnostic test into a health product that is valuable for routine healthcare from the end user's perspective.
Understanding the main principles of the EU CE certification process and national reimbursement systems is pivotal for research and development as well as successful market entry of photonic-based diagnostic tests.

APPLICATIONS/AI-DRIVEN BIOPHOTONICS – HEALTH: ADVANCED UNDERSTANDING OF CELL PROCESSES AND ORGAN FUNCTIONS

5 March // 9 - 10:30 a.m. // Grete Unrein Room
Chair: Christian Eggeling

Machine learning-assisted optical nanoscopy

Flavie Lavoie-Cardinal - Universitē Laval, Quēbec, Canada

With the advent of artificial intelligence (AI), smart microscopy strategies have emerged, enabling us to observe cellular processes in living brain tissues with unprecedented spatio-temporal precision. The integration of machine learning techniques to optical microscopy, and more specifically to super-resolution microscopy (nanoscopy), opened new possibilities to optimize image acquisition and analysis towards a better characterization of the molecular mechanisms underlying synaptic organization and remodelling [1,2]. We have developed AI-assisted microscopy approaches for: 1) quantitative analysis of neuronal protein organization in optical nanoscopy images [1,2,3], and 2) the optimization of image acquisition schemes, especially in living neuronal samples [4,5]. For instance, we developed a strategy based on a generative deep learning model that can be integrated within the image acquisition loop to guide the acquisition process, thereby minimizing the light exposure on living samples while still capturing the dynamics of neuronal processes at the nanoscale [6]. This allows us to perform time-lapse imaging of protein reorganization at the nanoscale in living cultured neurons. Ultimately, the development of data-driven microscopy is transforming our ability to discover and characterize rare phenomena that may influence synaptic connections and thus to discover new mechanisms influencing brain function in health and disease.

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Reconstructing brain tissue with light microcopy

Johann Danzl - Institute of Science and Technology Austria, Klosterneuburg, Austria

Brain tissue is a tantalizingly complex arrangement of neurons into an information processing network. Its cellular structure is too fine grained to be captured by conventional light microscopy, such that dense reconstruction of brain circuitry at synaptic resolution has been the exclusive domain of electron microscopy.
We have recently developed an optical super-resolution imaging/machine learning technology to reveal the cellular architecture and dynamics of living brain tissue at nanoscale detail (Velicky et al., Nature Methods (2023), DOI: 10.1038/s41592-023-01936-6). We have further established an extracellular labelling/super-resolution imaging approach to visualize brain tissue architecture across spatial scales in fixed tissues, including clinical specimens (Michalska et al., Nature Biotechnology (2023), DOI: 10.1038/s41587-023-01911-8).
Here, I will discuss our recent developments towards dense, synapse-level reconstruction of brain tissue with light microscopy, combining specifically engineered high-fidelity hydrogel expansion with high-speed, diffraction-limited imaging to achieve the resolution and signal-to-noise ratio required to trace and automatically segment even the finest of neuronal structures. This will give direct access to molecular information in brain tissue reconstructions in an easily adoptable manner, thus helping to shed light on fundamental questions of tissue organization and connectivity both in healthy and diseased brains.

Noise amplification and ill-convergence of deconvolution

Sjoerd Stallinga - Delft University of Technology, Delft, Netherlands

An important quest in the field of imaging is to devise instruments and methods to deliver the sharpest and most contrast rich images possible. Computational enhancement of raw images acquisitions are an important and broadly applied inroad to do so. This enhancement can be achieved via image processing steps such as filtering operations that are applied ad hoc, agnostic to the underlying physics of the image formation, or via learning based data driven approaches. Deconvolution, on the other hand, provides an estimate of the underlying object using statistical inference and a model of the image formation. The archetypical algorithm in this field is Richardson-Lucy (RL) deconvolution. An important advantage is that it enables reconstruction of out-of-band information, depending on the type of object that is imaged.

The application of RL deconvolution to practical imaging settings in astronomy or microscopy has brought to light that the algorithm converges slowly, if at all. Moreover, with increasing number of iteration steps an apparent noise structure builds up, originating from small perturbations of the input due to physical and/or numerical noise. In my presentation, I address the questions why RL deconvolution has a problematic convergence or why the procedure is so sensitive to noise, using a Cramēr Rao Lower Bound (CRLB) analysis. As the RL algorithm is a form of Maximum Likelihood Estimation for the ground truth object, a hypothetical well behaved optimum must have a lower bound on the precision of the estimate of the object, and this lower bound is the CRLB. I will show that the CRLB diverges and that hence the original assumption of a regular, well-behaved optimum must be false. It also intimately connects noise sensitivity and noise amplification to a lack of convergence of the iterative procedure. In the presentation I will also provide a review of existing and an outlook on new mitigation strategies for this problematic behaviour.

APPLICATIONS/AI-DRIVEN BIOPHOTONICS – HEALTH: CARDIOVASCULAR DISEASES

5 March // 9 - 10:30 a.m. // Clara and Eduard Rosenthal Room

Chair: Roberto Pini

Dissecting the role of structural remodelling on trans-scar conduction in arrhythmogenic mouse hearts by advanced optical methods

Leonardo Sacconi - University of Freiburg, Freiburg, Germany

Cardiac diseases often lead to severe structural remodeling of the heart, such as excess collagen deposition (fibrosis) and cellular misalignment, that can significantly impact cardiac electromechanical function and lead to arrhythmias. In this context, arrhythmogenic cardiomyopathy (ACM), an inherited heart disease, involves ventricular dysfunction, arrhythmia, and localized replacement of cardiomyocytes with scar tissue. Assessing the impact of minute structural remodeling on electrical dysfunction in whole organs is challenging due to the difficulty of performing high-resolution three-dimensional imaging over large volumes.

In this study, we developed a correlated multimodal imaging approach to investigate the structural basis of trans-scar electrical conduction in a mouse model of ACM, compared to wild-type (WT) controls (n=9/cohort).

After optical mapping of action potential propagation (APP) in Langendorff perfused hearts at different pacing rates, we transformed hearts into well-preserved, fully transparent organs using the SHIELD procedure optimized for cardiac tissue. We developed a high-throughput light-sheet mesoscope (called MesoSPIM) to reconstruct whole hearts with a voxel size of 6 micrometers in a single scan, imaging the myocardium from muscle autofluorescence and collagen depositions from elastic scattering signal. We quantified 3D myocyte orientation and fibrotic patches, generating an integrated computational model of organ's electrical activity. Our data indicate that ACM is associated with increased irregularity of the APP wavefront and with structural remodeling of ventricles, where fibrotic scars alter APP differently as the excitation frequency varies, but the role of this structural remodeling remains unclear. We suggest that combining our correlative imaging approach with APP simulations.

The intricate interactions between biophotonics, artificial intelligence, and inflammation

Kirsten M. Meiburger - DET - Politecnico di Torino, Turin, Italy

This talk will briefly explore the dynamic interplay between biophotonics, artificial intelligence (AI), and inflammation. Biophotonics facilitates non-invasive, high-resolution and functional imaging in the role of multi-spectral photoacoustic imaging. Integrating AI offers new tools to optimize and enhance photoacoustic imaging, specifically when considering photoacoustic tomography applications whose application in the clinics could be hampered by artefact-ridden images and time-consuming image reconstruction algorithms. Focus will be put on how photoacoustic image analysis and reconstruction, coupled with AI in a collaborative and synergetic manner, can contribute to advance biomedical research and precision medicine, facilitating the in-depth visualization and analysis of dynamic pathophysiological changes linked to disease progression. The talk aims to provide a basis to encourage discussion regarding the gaps and challenges in these fields, paying particular attention to the role that ethical artificial intelligence must play in the future regarding two specific aspects: (1) avoiding biases in quantitative biomedical optical imaging methods that have tended to be overlooked until recent years, such as skin tone; and (2) providing a robustness analysis in terms of explainability or uncertainty.

Biophotonics in the Era of Big AI

Andrea Barucci - Institute of Applied Physics "Nello Carrara" (IFAC), Council of National Research (CNR), Sesto Fiorentino, Florence, Italy

Biophotonics and Machine Learning (ML) have the potential to become a valuable tool in clinical applications. However, biophotonics data analysis with ML can show issues caused by the complexity, high dimensionality and reduced amount of data. These issues can prevent to understand the generalization performance of our system, precluding its application in clinical settings. The aim of my presentation is to make a journey through some of my Machine Learning applications, going from Radiomics up to Celestial Mechanics and Egyptology, focusing in particular on Biophotonics. I will try to outline the ubiquity of such methods in different fields, showing the strengths and weaknesses.

Data and software sharing, biobanks and virtual research environments will be discussed, in particular in the context of the projects Navigator, Optimised and ProCancer-I, where ML models have been developed integrating different kinds of data (clinical images and data, biophotonics sensors, etc.).

In the era of Big Artificial Intelligence, where every day newer ML models such as foundational models are available, Biophotonics must find its role.

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APPLICATIONS/AI-DRIVEN BIOPHOTONICS – HEALTH: WELLBEING

5 March // 11 a.m. - 12:30 p.m. // Ernst-Abbe Hall
Chair: Christian Huck

The next generation of medical imaging is spectroscopic.

Johannes Dominikus Pallua - Medical University of Innsbruck, Innsbruck, Austria

Over the past decade, cutting-edge spectroscopic imaging techniques have fueled remarkable progress in biomedical research. Collaborative efforts between the Medical University of Innsbruck and the Leopold Franzens University of Innsbruck (Tyrol, Austria) have brought to light the vast potential of these methods across diverse fields, including microbiology, pathology, forensic science, and clinical research. These studies underscore the transformative impact of advanced spectroscopic imaging techniques in biomedical research. Spectroscopic imaging technologies present precise and informative methods that promise to revolutionize the medical field. Ongoing research in these domains promises and actively contributes to revolutionizing medicine. Our research showcases the ever-expanding horizons of spectroscopic imaging techniques in medical diagnostics. It presents innovative approaches and explores their implications for addressing diverse medical challenges and advancing clinical research.

Miniaturized NIR spectrometers in food assessment and quality inspection: chemometric model interpretation

Justyna Grabska - University of Innsbruck, Innsbruck, Austria

Near-infrared (NIR) spectroscopy (800-2500 nm) has emerged as a major analytical tool offering versatility in wide-ranging applications. Its impact in practical applications multiplied with the advent of miniaturized spectrometers in the past decade. These cost-effective, portable instruments form particular synergy with the common advantages of NIR spectroscopy; rapid, non-destructive, and highly practical analytical solutions capable of delivering real-time/continuous analysis of multiple quality parameters simultaneously. These advantages are indispensable in controlling the quality and characteristics of products/processes in a multitude of industries.

These portable instruments have revolutionized quality control across application sector, including agriculture, food analysis, forensics, security, and manufacturing. In particular, miniaturized NIR spectroscopy pivotal role in food assessment and quality inspection, as the direct on-site analysis of the target property regardless of complex and diverse matrices, typical for food products, becomes feasible.

In this context, miniaturized NIR spectrometers offer unique and superior capabilities. However, these devices operate on diverse technological principles, resulting in variations in prediction performance and selectivity. As analytical framework in NIR spectroscopy relies on the training of machine learning/chemometric models, this instrumental difference introduces a new plane of specificity to the entire process.

This presentation explores how a deeper mechanistic understanding of NIR spectroscopy can optimize the applications. Simulation based on ab initio anharmonic methods unravels detailed structural fingerprint in the intrinsically complex, highly convoluted NIR spectra. Specifically, the physical interpretation of NIR bands opens up new avenues for profiling the analytical potential of miniaturized sensors. These miniaturized sensors often capture only a fragment of spectral information from samples, making the detailed understanding of chemometric models crucial for extracting valuable insights.

By dissecting chemometric models and augmenting them with interpreted information, we demonstrate how this approach enables a comprehensive assessment of sensitivity and selectivity, particularly against specific compounds or chemical moieties.

Unveiling the synergy of NIRS and enrichment technologies: A success story of in-sorbent based detection and quantification strategies

Christian Huck - Leopold-Franzens University, Innsbruck, Austria

This presentation aims to captivate the applicability of in-sorbent detection, where near-infrared spectroscopy (NIRS) converges with enrichment technologies. For this purpose, information regarding the combination of several sophisticated analytical enrichment techniques with NIRS to further explore and develop this synergistic approach are presented. Investigations according to used materials, commercial or self-made, composition, organic or inorganic and applied analytical methodologies are discussed. As this presentation concludes, the combination of these techniques further expands the applicability of NIRS and moreover tries to solve the long-standing issue of the comparably low sensitivity regarding this vibrational technique.

APPLICATIONS/AI-DRIVEN BIOPHOTONICS – HEALTH: FURTHER TOPICS

5 March // 11 a.m. - 12:30 p.m. // Grete Unrein Room

Chair: Kishan Dholakia

The ubiquity of fluorescence spectroscopy and imaging in biomedicine

Laura Marcu - University of California, Biomedical Engineering, Davis, USA

Integrating Orbital Angular Momentum in AI-driven Biophotonics: Enhancing Health

Igor Meglinski - Aston University, Birmingham, UK

We explore the potential of structured vortex laser beams, known also as shaped light with orbital angular momentum (OAM), for diagnosis of cells and cells cultures, as well as for quantitative characterization of biological tissues. The structured vortex beams contains a spin contribution, conditioned by the polarization of the electromagnetic fields and an orbital contribution, related to their spatial structure. When the shaped light propagates in a homogeneous transparent medium, both spin and orbital angular momenta are conserved. In order to study a conservation of spin and orbital angular momenta of the shaped light propagation in a homogeneous transparent medium we have built a Mach-Zehnder-like interferometer featuring spatial light modulator (SLM) for generating Laguerre-Gaussian (LG) light beams with different momenta. The LG beam passes through a tissue sample and the interference with reference plane wave is detected on the camera. We show that when the LG beam propagates through normal and cancerous tissue samples the OAM is preserved with the noticeably different phase shift – twist of light. We also demonstrate that the twist of light is up to ~ 1000 times more sensitive to the refractive indices changes within the tissue samples and, therefore, has a high potential to revolutionize the current practices of tissue diagnosis, e.g. histology examination. The results of our experimental studies are well agreed with the results obtained with newly developed by Monte Carlo code developed in-house. Finally, we conclude that the application

of OAM for biomedical diagnosis offers fascinating opportunities for both new fundamental biological studies and practical clinical applications. This approach promises early detection, personalized treatments, improved patient care, and outcomes, marking a significant leap in integrating Biophotonics and AI for global healthcare advancements.

Improving IVF success with advanced photonics

Kishan Dholakia - University of Adelaide, Adelaide Australia

Embryo quality is a crucial factor affecting live birth outcomes. However, an accurate diagnostic for embryo quality remains elusive in the IVF clinic. Exploiting advanced optical imaging can assess the embryo in 3D and determine its metabolic rate and other physical parameters. This may ultimately prove to be a new multimodal diagnostic approach for embryo health.

In this talk I will describe the use of a range of advanced photonics-based approaches as a step towards the understanding of the development of the pre-implantation mammalian embryo [1-4]. The ultimate goal is to improve IVF outcomes.

Cellular metabolism is a key regulator of energetics, cell growth, regeneration, and homeostasis. The endogenous metabolic cofactors, nicotinamide adenine dinucleotide (phosphate) (NAD(P)H) and flavin adenine dinucleotide (FAD) can be imaged through their autofluorescence. By performing this with hyperspectral imaging at subcellular resolution may assist in determining embryo viability in a clinical setting. Such hyperspectral imaging can be used to determine the ploidy status of the embryo [1]. By using light sheet imaging, we can extend this imaging to 3D [2]. Separately digital holographic microscopy (DHM) can be used to measure spatio-temporal changes in refractive index during the development of the embryo that are reflective of its lipid content. Accumulation of intracellular lipid is known to compromise embryo health thus making this a useful approach for diagnosis [3]. Overall, advanced optics adds useful, multimodal information for IVF success and can be gentle enough to not effect viability [4].

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APPLICATIONS/AI-DRIVEN BIOPHOTONICS – HEALTH: NEURO-DEGENARTIVE DISEASES

5 March // 11 a.m. - 12:30 p.m. // Clara and Eduard Rosenthal Room
Chair: Francesco Pavone

Large-scale imaging and feature extraction using advanced high-resolution microscopy techniques

Giacomo Mazzamuto - National Research Council – National Institute of Optics (CNR-INO), European Laboratory for Non-Linear Spectroscopy (LENS), Sesto Fiorentino, Italy

Advanced microscopy techniques, such as Light-Sheet Fluorescence Microscopy (LSFM) and Two-Photon Fluorescence Microscopy (TPFM), enable three-dimensional imaging of biological tissue at high resolution. These techniques have gained popularity within the neuroscience community for their capacity to provide detailed insights into the intricate structures of neural tissue.

In this talk, I will present the capabilities of the Biophotonics lab at CNR-INO and LENS, along with some of the latest results regarding the investigation of human and mouse brain tissue using high-resolution 3D microscopy. The lecture will particularly highlight our expertise in the three main areas that are necessary for the successful operation of these advanced microscopy techniques: 1. tissue clearing and staining, 2. custom development of advanced optical setups, and 3. development of a custom image processing pipeline.

Image processing in particular poses a significant challenge in this type of microscopy due to the large amounts of data produced when imaging large volumes at high resolution, often reaching several terabytes per sample. The image processing pipeline includes volumetric image stitching, compression, and various transformations. Moreover, to extract biologically meaningful quantities – such as cell counts – from these extensive datasets, automatic techniques based on artificial neural networks are needed.

The imaging campaigns showcased in this talk encompass the investigation of whole mouse brains and large slices of human brain cortex, including specimens from subjects with neurodegenerative diseases. It is then shown how the whole imaging and post-processing pipeline enables the extraction of quantitative information and the investigation of the layer-specific organization of the cerebral architecture.

AI-driven microscopy for brain functional connectivity reconstruction

Francesco Saverio Pavone - University of Florence, Sesto Fiorentino, Italy

The tremendous technological improvement in both optical methods and genetically encoded indicators and actuators, combined with the tiny and transparent larval zebrafish as an animal model, opened the way to experimental possibilities that appeared prohibitive just a couple of decades ago: the all-optical recording and perturbation of the electrical activities of large populations of neurons spanning an entire vertebrate brain. With respect to conventional electrode-based electrophysiological studies, these all-optical approaches dramatically expand the number of possible neuronal targets to interact with, thus posing novel and tough challenges in terms of throughput of combinatorial possibilities when handling experiments. Here, we present a custom microscope intended for the all-optical dissection of brain physiology in zebrafish larvae. The system is composed by a two-photon (2P) light-sheet microscope for high-speed volumetric functional imaging, a light-targeting system employing acousto-optic deflectors for selective 2P 3D optogenetic stimulation and a machine learning-based software. The experimenter decides the target of the stimulation. The software analyzes and interprets whole-brain functional data evoked by the photostimulation, providing the experimenter with a set of coordinates for novel promising targets of a second stimulation round. By iteratively running the system, it is feasible to rapidly reconstruct the efferent functional connectivity of selected neuronal circuitries, thus dissecting the hierarchy of the network. The system we devised enables an unprecedented experimental scenario in the investigation of the physiology and pathology of the vertebrate brain.

ECOSYSTEM – FROM RESEARCH TO MARKETS

5 March // 2 - 3:30 p.m. // Grete Unrein Room
Chair: Markus Wilkens

Patenting at the Heart of IT: AI & MedTech

Felix Grasbon - Grättinger · Möhring · von Poschinger Realpatent Patentanwälte, Starnberg, Germany

Patent trends and (European) patent practice in the dynamic intersection of artificial intelligence and medical technology. The global patent landscape and its development in medical technology are illustrated with a special focus on patenting of AI implementations. We look at regions, companies, and key technologies, as well as changes in recent years. For example, China's IP activity should prompt Western players of all sizes to increase their IP awareness. As inventors, patent attorneys and examiners worldwide gain more and more experience in handling AI-related inventions, we provide insights into how applied AI in the field of medical devices can be protected by explaining the basics of the patent system and the key aspects with respect to computer-implemented inventions, and specifically machine learning applications.

MedPhab - Photonics pilot line for accelerated product development

Jussi Hiltunen - VTT Technical Research Centre of Finland Ltd, Espo, Finland

The medical device industry is a significant opportunity area for photonics technologies. Photonics-based medical technology and life science applications have shown substantial growth driven by the trends of minimally invasive surgeries, in-vitro & in-vivo diagnostics, drug development and biotechnology. However, the production environment in photonics can be challenging. Photonic devices and products are often heterogeneous in nature whilst there is also a fragment market offering and this can result in delays in product development. Also, for the end-user companies it is not obvious which technology can provide the best solution due to rapid advancements of photonics. The widespread use of photonics in scattered ecosys-

tems therefore presents major challenges for both end-user companies and manufacturers. To accelerate the uptake of photonics technologies, MedPhab pilot line was established with its low barrier open access model focusing on the high impact medical application domain. The model is supported by the modularised fabrication and established production libraries. Depending on the customer needs and required TRL, the work is distributed between ISO13485 certified companies and RTOs. The possibility to realise devices at different TRL using same/compatible production equipment can greatly accelerate time to market by eliminating the need to redevelop processes, reprogram equipment, or retrain personnel. The participation of companies with ISO13485 standardized manufacturing ensures the seamless transition from pilot line production to up-scaled production without a need for changing service providers.

Navigating towards trustworthy AI

Lena Kästner - University Bayreuth, Institute for Philosophy, Bayreuth, Germany

Artificial intelligence (AI) continues to permeate various aspects of our modern lives. Contemporary machine learning based systems are ubiquitous; they range from face recognition in our smartphones to spam filters in our email to media creators all the way to decision support systems for judges, pilots and doctors. This prevalence of AI raises legal, moral and ethical questions alike which typically relate to a system's reliability, safety, fairness, and trustworthiness. This talk delves into the multifaceted question of trustworthy AI systems might be realized. What exactly does it take for a system to be considered trustworthy? What options do users have to assess a system's trustworthiness? And how can developers work towards making opaque machine learning based systems trustworthy? As a starting point for an interdisciplinary discussion, I suggest that one avenue towards trustworthy AI leads via building mechanistically interpretable models of opaque AI systems.

Biopharmaceutical Value Chain

Marcus Rieker - HORIBA, Oberursel, Germany

TRANSLATION – BEST PRACTICE EXAMPLES

5 March // 4 - 5:30 p.m. // Ernst Abbe Hall

Chair: Antonio Castelo

High performance miniaturized Raman systems for biological applications

Oleksii Ilchenko - Lightnovo, Birkerød, Denmark

From science to start-up: Rapid Histology of Fresh Tissue Samples Using a Clinical-Compatible Stimulated Raman Imaging Device

Tim Hellwig - Refined Lasers Systems, Münster, Germany

Bringing microscopy through a single-fibre to biologists

Patrick Westermann - DeepEn, Jena, Germany

APPLICATIONS/AI-DRIVEN BIOPHOTONICS – HEALTH: PREVENTION & EARLY DIAGNOSIS

6 March // 9 - 10:30 p.m. // Ernst-Abbe Hall
Chair: Francesco Baldini

Graph representation learning and biophotonics

Pietro Liō - University of Cambridge, Department of Computer Science and Technology, Cambrdige, UK

The potential and pitfalls of artificial intelligence techniques in tumour detection

Sara Colantonio - National Research Council of Italy, Institute of Information Science and Technologies, Pisa, Italy

Cutting-edge AI technologies have the potential to enable new models of care, improve disease prevention and enhance quality of life. These advances can pave the way for increasingly personalised, accessible, efficient and sustainable health and care systems.
The field of radiology holds great promise for the use of artificial intelligence and image processing methods. AI-powered applications can help radiologists optimise their diagnostic workflow, as they have the potential to improve the objectivity and reproducibility of radiological assessments. This is particularly beneficial in high-stress environments where sustained attention over long periods of work is a challenge. By performing tasks tirelessly and consistently, AI-based applications can reduce the burden on clinicians, by helping them prioritizing cases that demand heightened scrutiny, such as in cancer screenings where expeditious assessment of suspicious cases is vital.
Furthermore, the integration of machine learning and data science tools proves fruitful in the identification and consistent measurement of new biomarkers, facilitating, for instance, the prediction of tumour aggressiveness. Ultimately, AI tools can prove indispensable in bolstering resources for less well-equipped facilities, offering techniques to enhance data resolution.

These instances represent a mere glimpse into the potential benefits of AI methodologies in the field of radiology.
Nevertheless, the use of AI technologies in clinical practice is still limited. Recent surveys have shown that many clinicians believe that AI solutions could improve their specialty. However, the vast majority of them have never used any AI-powered applications in their daily practice, and only a few consider themselves to have excellent knowledge of the field. Barriers to the adoption of new technologies include challenges to human autonomy, accountability, and liability, as well as potential biases and risks. In addition, users may experience dissatisfaction with user interfaces and find the effort and cognitive load required to use the technology excessive. Overall, there is a reported lack of trust in AI-powered tools, which may be related to a lack of understanding about their assumptions, limitations, and capabilities. High-quality scientific foundations, technical robustness, and responsible development are the only ways to overcome these concerns.
This talk will provide an overview of the most recent advancements in the field, as well as recent international initiatives to ensure AI trustworthiness, such as the FUTURE-AI guidelines.

Towards Early Diagnosis of Colo-Rectal Cancer

Peter E. Andersen - Technical University of Denmark, Kongens Lyngby, Denmark

Colorectal cancer (CRC) is the second most common cause of cancer death in Europe, yet survival rates rise dramatically when caught early. A contributing factor is that current colonoscopy, i.e., white light video or optical narrow band imaging, is inadequate for in-vivo detection and characterisation of the various types of (pre-)cancerous lesions found in the colon. Point-of-care, real-time polyp diagnosis and image guided intervention has the potential to save huge healthcare costs by enabling early onset of treatment; thus reduced recurrence rate, by improving interval screening, and by reducing pathology costs incurred during colonoscopy.
A complete, reliable optical diagnosis is sensitive to morphological and biochemical changes. Unfortunately, no single optical method provides both. PROSCOPE provides unique combination of label-free, non-ionizing, proven optical imaging modalities that provides higher sensitivity and specificity compared to current colonoscopy thus enabling a step-change in point-of-care management of CRC. PROSCOPE develops and integrates recent advances in optical imaging and optical probe technology into one platform. A leading medical device manufacturer and clinicians are involved at every stage of the development and validation. In this presentation, an overview of the current status of the multimodal system development is given, including examples of technologies.

APPLICATIONS/AI-DRIVEN BIOPHOTONICS – HEALTH: CANCER THERAPY (ROBOTICS)

6 March // 9 - 10:30 p.m. // Grete Unrein Room
Chair: Laura Marcu

Guidance for Cancer Resection with AI and Surgical Vision

Stamatia Giannarou - Imperial College London, Faculty of Medicine, Department of Surgery & Cancer, London, UK

Surgery is undergoing rapid changes driven by recent technological advances and our on-going pursuit towards early intervention and personalised treatment. The future of surgical oncology is the integration of novel intraoperative imaging techniques to enable in vivo-in situ diagnosis and therapy and allow for more accurate tumour margin delineation. The main challenges to such integration are the intraoperative surgical navigation, the scanning of large tissue surfaces with imaging probes, the tissue characterisation and the safety during resection by protecting important anatomical regions and healthy tissue.
In this talk, I will present an intraoperative vision system for surgical navigation and real-time tissue characterisation during robot-assisted neurosurgery to improve both the efficacy and safety of tumour resections. The focus will be on the recovery of 3D morphological structures in the presence of tissue deformation, the efficient robot-assisted tissue scanning with imaging probes and the tissue characterisation for on-line diagnosis support.

Perspectives on Implementing Biophotonic Technologies in the Operating Room for Head and Neck Cancer

Andrew Birkeland - University of California, Davis, USA

Head and neck cancer is the 6th most common cancer worldwide. Surgery is a key component in the treatment of head and neck cancer. Removing all cancer with clear margins is one of the strongest predictors for survival in head and neck cancer. However, appropriate surgical excision with clear margins remains challenging. Intraoperative imaging techniques are gaining research interest to help delineate appropriate surgical resection of head and neck cancers. Here we will discuss the current state of research technologies in intraoperative imaging in head and neck cancer, with a focus on biophotonic technologies. We will discuss intraoperative considerations from a surgeon's perspective on clinical gaps and needs, and opportunities for integrating such technologies into the clinical workflow. We will address potential opportunities for further growth and investigations into clinical implementation of biophotonic technologies in the operating room, and in particular for head and neck cancer surgeries.

Digital Surgery and Surgical Robotics

Jonathan Sorger - Intuitive Surgical, Sunnyvale, USA

Recent advances in GPU architectures and the proliferation of cloud computing + software tools have spurred interest in artificial intelligence and machine learning algorithms applied to the space of surgical robotics.
While these advances are certainly exciting, they are simply tools used in the larger field of digital surgery, a loosely defined term which encompasses data capture & analytics, decision-making support, smart instrumentation, advanced visualization techniques, improved connectivity and levels of autonomy.
By placing a computer between the surgeon and patient, surgical robotics enhances many aspects of digital surgery, as the sheer amount of data collection possible facilitates the application of both supervised and unsupervised algorithms. This has been the case in terms of skills analysis, predictive outcomes as well as robot engineering design.
While different levels of autonomy exist in addition to several successful examples in the medical space, challenges remain in terms of autonomy in surgical robotics, as anatomic variability as well as unpredictable situations frequently arise during surgery. Training data sets are not as well-developed as those in the autonomous car industry, nor are in-vivo sensing technologies, which has seriously hampered progress in the field.

Multi-parametric standards for quality control and performance assessment of fluorescence molecular imaging systems

Dimitris Gorpas - Helmholtz Center Munich / Technical University of Munich / Central Institute for Translational Cancer Research, School of Medicine and Health, Munich, Germany

Fluorescence molecular imaging (FMI) and endoscopy (FME) are emerging as technologies with great potential to guide surgical and endoscopic interventions and to provide earlier, faster, and personalized diagnosis in oncology. In tandem with the recent advances in the development of novel tracers, their clinical validation is currently assessed under numerous clinical trials worldwide. The recent approvals by the US Food and Drug Administration of approximately 20 fluorescence-guided clinical imaging systems, as well as three tracers for surgical guidance, i.e. 5-aminolevulinic acid for patients with suspected high-grade gliomas, hexaminolevulinate for use in non-muscle-invasive bladder cancer, and pafolacianine for intraoperative imaging of folate receptor-positive ovarian cancer are a promising result of the ongoing efforts.

However, FMI and FME still present challenges that can confound real-time decision making for disease management and/or treatment. Importantly, the markedly different systems hurdle the repeatability of measurements, the unbiased readout interpretation, and their wide acceptability as “red flag” techniques for cancer detection. To that end, the first efforts for standardization of systems and procedures start to appear in literature and guidelines are suggested by different study groups.

Herein we discuss some of these efforts and guidelines, as well as the work implemented by our group for the development of multi-parametric, composite standards to perform quality control and performance assessment of FMI and FME systems. We also discuss specific designs that are linked to various acquisition and performance parameters, as well as data analysis approaches to ensure optimal and objective quantification of the various system parameters.

The discussed standardization framework may accelerate the clinical translation of fluorescence molecular imaging for surgical guidance and endoscopy and can steer further development in the area of robotic interventions. Finally, the possibility to perform quality control through a fluorescence standard is expected to be pivotal for robotic assisted fluorescence molecular imaging, where the employed scopes are prone to performance degradation due to the use-sterilization cycles.

APPLICATIONS/AI-DRIVEN BIOPHOTONICS – HEALTH: CONTINUOUS MONITORING

6 March // 9 - 10:30 p.m. // Clara and Eduard Rosenthal Room
Chair: Werner Mäntele

Unfolding proteins on the fingertip - a mid-IR lab-on-a-chip for real-time reaction monitoring of liquids

Borislav Hinkov -Silicon Austria Labs, Villach, Austria; TU Wien, Vienna, Austria.

The measurement of molecules in liquid and gas phase is nowadays often conducted in the mid-IR spectral range, where many molecules show their fundamental, i.e. strongest, absorptions. Together with the specific spectral fingerprint of every molecule, this enables a very sensitive and selective molecule detection. However, many experiments are still using big and bulky equipment such as Fourier-transform infrared (FTIR) spectrometers, often limiting their operational capabilities to lab-scale configurations or preventing interesting real-time measurements such as in dynamically changing fluids or in in-situ liquid experiments. Fortunately, there is a solution which can be found in the emerging quantum- and interband-cascade (QC/IC) technology. These novel types of devices allow addressing the mid-IR spectral range with highly powerful laser sources and sensitive detectors, which are moreover small and compact. Furthermore, they can be combined with passive mid-IR elements (waveguides, modulators, ...) into functional monolithic photonic integrated circuits (PICs). Such fingertip-sized PICs can then be used in unprecedented experimental configurations.

In this work, we demonstrate the realization of a QC-based monolithic PIC in a lab-on-a-chip (LOC) configuration and its application in real-time reaction monitoring of protein dynamics. In particular, the temperature-dependent conformational changes of the model protein bovine serum albumin (BSA) in D2O are monitored. By showing in-situ operation inside the beaker with the protein solution and micro-liter scale liquid probing, both in direct contact of the liquid with the integrated plasmonic sensing section of the LOC, two unprecedented key features are demonstrated.

In additional work, we show the integration of further functionalities into the LOC including surface passivation for a more robust plasmonic sensing section, surface functionalization for

enhanced molecule probing and the integration of novel mid-IR materials and concepts for more complex PIC configurations like fully chip-scale integrated Mach-Zehnder interferometers (MZIs) based on on-chip mode guiding and re-directing capabilities.

Non-Invasive Blood Glucose Measurement with Infrared Quantum Cascade Lasers and Photothermal Detection

Sergius Janik - DiaMonTech AG, Berlin, Germany

Around 530 million people worldwide suffer from diabetes, with increasing tendency. Diabetes can presently not be cured, but managed by strict control of blood glucose and adaptation of food intake, physical activity, medication or insulin injection. The current method of blood glucose control involves pricking and analysis of a drop of blood by enzyme-based test strips fitting into a glucometer. This intermittent and invasive measurement is painful and unpleasant and thus by far not performed frequently enough; it only provides a snapshot of the blood glucose level at a time. Recently, minimally invasive sensors have been introduced that use a flexible needle in the interstitial fluid (ISF) of skin and are used for quasi-continuous monitoring.

DiaMonTech has developed a photonic technique based on infrared quantum cascade lasers (QCL) and photothermal detection for a truly non-invasive glucose measurement. This technique targets a glucose signature in the mid-infrared in the spectral range of approx. 8-11 µm caused by the vibrations of the glucose molecule (mainly –C-O- stretching and –O-H bending modes). This signature is highly specific for glucose in terms of a "glucose fingerprint" that can be used to distinguish glucose from other molecules in skin, and thus warrants the specificity required for a reliable glucose sensor. The proprietary photothermal detection senses the tiny amount of heat deposited from glucose molecules in skin after QCL excitation of vibrational modes from glucose molecules immediately followed by thermal relaxation.

The talk presents the basic physics of the technology and the development of a table-top device for clinical validation of this novel non-invasive glucose measurement. It describes the miniaturization to a smartphone-size portable device as a daily companion of the diabetes patient. Data evaluation algorithms and calibration routines are discussed. Clinical tests are reported that reveal a precision close to early minimally-invasive devices.

SERS-based detection schemes in biomedical application

Dana Cialla-May - Leibniz Institute of Photonic Technology / Friedrich Schiller University, Jena, Germany

Raman spectroscopy is a powerful analytical tool in biomedical application schemes; however, its limitation is associated with the intrinsic weak Raman effect. This is overcome by applying powerful plasmonic nanostructures creating the surface enhanced Raman spectroscopy (SERS) technique. SERS is applied to identify and estimate trace concentration of biomolecules such as drugs and its metabolites or biomarker even in complex matrices. [1, 2] The SERS technique was applied to estimate the antibiotic ciprofloxacin in pharmaceutical formulations. In the case of simple matrix compositions, e.g. sodium chloride infusion solutions, Raman spectroscopy can be applied in the required concentration range. For formulations with high Raman background signal, a dilution by 1:5000 was applied and the recorded SERS spectra were only dominated by the contribution of the target ciprofloxacin, which is associated with the strong affinity of this drug towards the metal sensing surface. [3] Furthermore, we illustrated the SERS-based detection of pyrazinoic acid (POA), a metabolite of the tuberculosis-relevant prodrug pyrazinamide (PZA). To be specific for POA, gold nanoparticles equipped with a Prussian blue modification were applied, complexing the POA molecules via Fe (II). This scheme has a high potential in assessment of PZA resistance in M. tuberculosis bacteria, as only sensitive bacteria convert PZA into POA. [4] To illustrate the potential of SERS in therapeutic drug monitoring, the antibiotic ceftriaxone was spiked in fresh blood plasma samples as well as microdialysates and the role of proteins within this detection scheme is discussed. In microdialysate samples, detection down to 1.4 µM is achieved. [5] Finally, we studied the SERS signature of saliva to verify the detection of salivary biomarkers, i.e. interleukin-8 and lysozyme by combining SERS with molecular dynamics simulations. [6]

References:

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2. Liu et al., TrAC 164 (2023) 117094.
3. Liu et al., Talanta, 250 (2022) 123719.
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5. Liu et al., Talanta 271 (2024) 125697.
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APPLICATIONS/AI-DRIVEN BIOPHOTONICS – AGRICULTURE/FOOD

6 March // 2 - 3:30 p.m. // Ernst-Abbe Hall
Chair: Chris van Hoof

Opportunities of Photonic Integrated Circuits in AgriFood

Mark Ventile - imec / OnePlanet Research Center, Nijmegen Netherlands

PHOTONFOOD - Flexible mid-infrared photonics solutions for rapid farm-to-fork sensing of food contaminants

Achim Kohler - Norwegian University of Life Sciences, Ås, Norway

Analytical techniques for the measurements of chemical and microbial contaminations along the food chain require detection levels in the ppb range. A direct measurement of contaminants at theses concentrations in a food matrix is not possible by any photonics principle. The PHOTONFOOD project has received funding by the European Union's Horizon 2020 research and innovation programme (grant agreement No. 101016444) and is part of the PHOTONICS Public Private Partnership to overcome this barrier by a ground-breaking solution that integrates innovations in smart paper-based sample pre-treatment for separation and pre-concentration of the target analyte, mid-infrared (MIR) sensing, and advanced data analysis. Mid-infrared (MIR) spectroscopy has proven to be the most reliable and broadly applicable spectroscopic method for detection, characterization and quantification of chemical and microbial contamination. To transform MIR sensing from existing lab solutions into a portable solution to broad usage in the food chain, PHTONFOOD aims to develop novel infrared light sources, specifically interband cascade light emitting diode (IC-LED), and interband and quantum cascade lasers (ICL/QCL). The new light sources cover narrow ranges of the mid-infrared range. Their band width and emission range need to be adjusted to the target contaminant to be detected and the requirements for standardization of the measured signal. The aim of this presentation is to disseminate the general results of the PHOTONFOOD project and particular the challenges that are related to data analysis of the data obtained with the narrow band light sources in the mid-infrared range of the electromagnetic spectrum.

Multi-analyte, configurable biophotonics lab-on-chip platforms for on-the-spot food safety controls

Alessandro Giusti - CyRIC Ltd, Nicosia, Cyprus

There is an increasing need for miniaturized sensors providing simultaneous access to diverse chemical & biochemical information, required in various applications including food safety controls at various points of the farm-to-fork value chains. Currently, food safety inspections are based on sampling random batches using laboratory techniques, which may require up several days before getting results. The time and cost per analysis leads to reduced checks and thus elevated risks.
Novel biophotonics sensors, capable of simultaneously, cost-efficiently and quickly (within few minutes) detecting multiple contaminants of interest are being developed by CyRIC and its collaborators to address the aforementioned need. Two different approaches are being followed, currently laying at different technology readiness levels.
The first one (GRACED system) is a novel ultra-compact, cost-effective, plasmo-photonic bimodal sensor platform with on-chip light generation suitable for farm-to-fork applications. The sensing platform is part of a holistic, modular solution that exploits unique engineering designs, Internet-of-things (IoT) concepts and advanced data analytics, for the early detection of contaminations in the F&V value chains. The first operational prototype shows highly promising results. The bimodal SiN devices currently in fabrication are simulated to reach up to 12,000 nm/RIU. SU8-based bimodal sensors are also under development, expected to achieve about 11,000 nm/RIU.
The second one (MultiLab) exploits the know-how gained in the development of the GRACED system but approaches the sensing problem in a different way. It is based on a plasmonic augmented, Arrayed Waveguide Grating (PA-AWG) sensing module, developed on a Si3N4 photonic platform for true & scalable multiplexed detection. Scalability in multiplexing can reach unprecedented levels without scaling the readout complexity and respective assembly

costs. An array of differently functionalized aluminium plasmonic sensing elements will be integrated in the same AWG channel array in a Si3N4 waveguide-based PIC platform enabling simultaneous detection of proteins, miRNA and microorganisms (bacteria, viruses). Artificial intelligence (AI) will be exploited for analysing the novel PA-AWG sensor module outcome patterns and provide accurate measurements.

APPLICATIONS/AI-DRIVEN BIOPHOTONICS – HEALTH: OPTICAL DIAGNOSTICS

6 March // 2 - 3:30 p.m. // Grete Unrein Room
Chair: Paul French

Spectrally-resolved imaging in vivo -providing surgical guidance using vision and robotics

Daniel Elson - Hamlyn Centre for Robotic Surgery, Department of Surgery and Cancer, Imperial College London, UK

Strategies for the acquisition of spectrally-resolved data in human studies will be discussed. This includes the use of wide-field multispectral imaging, as well as spectroscopic modalities such as diffuse reflection spectroscopy and spectrally resolved fluorescence. While spectroscopy will be shown to provide high diagnostic accuracy, including in vivo, the ergonomic and visual limitations of these instruments will be shown as significant barriers to their use in surgery. The use of computer vision techniques for tracking of these devices and image-based contextualization will be presented as a potential solution. In addition, the use of commercial or custom-built surgical robotics systems can play a role in data acquisition and display. Finally, multispectral imaging data from 47 neurosurgery patients will demonstrate how combined spatial and spectral analysis can allow images to be segmented into multiple clinically-relevant classes.

From Technology to Discovery: Deeper, Faster, and Colorful Photoacoustic Imaging in Life Sciences

Junjie Yao - Duke University / Duke University School of Medicine, Durham, USA

Photoacoustic imaging (PAI) is an increasingly powerful technique for multi-scale anatomical, functional, and molecular imaging by acoustically detecting the optical absorption contrast in biological tissues. In PAI, a short-pulsed laser beam is used to illuminate the tissue, generating a tiny but rapid temperature rise and resulting in the emission of ultrasonic waves through thermoelastic expansion. The wideband ultrasonic waves are then detected to create high-resolution tomographic images that map the tissue's optical absorption.

In my talk, I will focus on several technological advancements in PAI that have collectively enabled fast, deep, and high-sensitivity biomedical applications and discoveries in life sciences, such as functional stroke imaging, drug testing, cancer detection, and interventional therapy. First, PAI has overcome the penetration limit by utilizing advanced internal light delivery techniques, allowing for super-deep (>10 cm) imaging. This breakthrough has extended the applicability of PAI to internal organ imaging in large animal models and humans. Second, innovative scanning technologies and deep-learning models have significantly accelerated PAI, enabling imaging speeds that are more than 1000 times faster while maintaining a large field of view and high spatial resolution. This enhancement facilitates the monitoring of highly dynamic biological processes at the microscopic scale, such as functional brain activities and glassfrog transparency. Third, through the use of novel fabrication technologies in optics and acoustics, miniaturized PAI systems have been developed. These handheld, wearable, and head-mounted imaging devices offer high spatial-temporal resolutions and high throughput, providing greater flexibility and accessibility in imaging applications. Lastly, PAI has greatly benefited from the genetically-encoded switchable or tunable near-infrared photoacoustic-specific probes. By incorporating these probes, the sensitivity and specificity of PAI have been improved by more than 1000 times, enabling highly sensitive detection of malignant cancer, tissue hypoxia, and neuronal activities.
By highlighting these technological advancements, my talk aims to update the recent progress made in PAI and its potential for a wide range of biomedical applications in life sciences.

STORM for diagnosis of kidney disease as well as ongoing work on cancer pathology tools

Paul French - Imperial College London, UK

APPLICATIONS/AI-DRIVEN BIOPHOTONICS – HEALTH: CANCER THERAPY (PDT & SURGERY)

6 March // 4 - 5:30 p.m. // Grete Unrein Room
Chair: Carsten Philipp

Interstitial Photodynamic Therapy – The Munich Experience

Ronald Sroka - Laser-Forschungslabor of LIFE-Center at Department of Urology at Hospital of University of Munich, Munich, Germany

This lecture gives an introduction about the application of photoactive drugs and their clinical use for cholangiocarcinoma, prostate cancer and in neurosurgery. Besides the medical needs, requests and boundary conditions, the physics and technical research and developments will be presented. Preliminary study results as well as the potential of optical dosimetry concepts based on light-tissue interaction and light-photosensitizer interaction are included summarizing the latest developments in this field.

Topical and systemic PDT – clinial experiences in NMSC – a bedside view

Carsten Philipp - Consultant Lasermedicine, Berlin, Germany

Skin is the largest organ of the human body. It is easy accessible for topical application of drugs and light dosimetry, due to the rather flat appearance in a first approximation. Furthermore, a larger number of skin diseases cover larger areas or show multifocal appearance, which favors regional or large field therapies and impedes surgical interventions. As scar formation is another unwanted result of surgery but less frequently seen in PDT, the widespread use of PDT in dermatology is a necessary consequence.
Since the introduction of ALA or MAL as precursor drugs topical PDT with PPIX has been developed into a reliable and effective tool for the treatment of superficial basal cell carcinoma (BCC) or Bowen's disease (MB) and actinic keratosis. This is even more important as

the incidence of those lesions shows a significant increase during the last decade and an even stronger increase must be expected in the future. The typical fluorescence of PPIX may also be used for fluorescence diagnostic and control of therapy and is another advantage. Overtreatment is unlikely, as PPIX shows a “bleaching” with subsequent decay of ROS-generation during the light exposure. A combination with OCT for tumor demarcation and depth measurement has shown to be applicable and helpful.

Pain during light exposure is one of the limiting factors for topical PDT. In a prospective control study, a dosimetry concept for pain reduction employing an escalating light fluence rate, first described by Nathalie Zeitouni et al.(1) was confirmed. Since then, we use this protocol with good patient acceptance and clinical results.

Nevertheless, topical PDT is only effective in some tumor types and thickness of the tumors is crucial as penetration of the drug (ALA or its derivatives) and conversion into PPIX is the limiting factor. In larger volumes and other tumor entities systemic PDT with intravenously applied photosensitizers (PS) offer advantages. As photosenzitation of skin in general is one of the typical features that come along with systemic PS, a differentiated light dosimetry becomes much more important. Shielding of non-diseased sites, interval between PS administration and light application, light dose and way of application (surface application or interstitial), single or repeated exposures are examples for the numerous variables in light application that may be applied.

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Fluorescence Lifetime Imaging for the real time diagnosis of lung cancer

Ahsan Akram - University of Edinburgh. Edinburgh, UK.

Non-small cell lung cancer (NSCLC) is the leading cause of cancer death with 1.8 million deaths annually worldwide. Early detection and intervention is crucial, however, current strategies for suspected cancers often rely on months of interval imaging, leading to cancer progression, delays in diagnosis and worse outcomes. During interventions like bronchoscopy, a targeted biopsy can also take days or weeks, further delaying diagnoses. With impending national lung cancer screening programs, this problem will worsen, straining healthcare resources and increasing patient anxiety.

Our approach and vision for this challenge is by enabling early intervention and immediate cancer diagnosis through in vivo microscopy, using a fibre-based translational fluorescence lifetime imaging (FLIM) system. FLIM measures the decay of light emitted by autofluorescent molecules. At the University of Edinburgh we have developed a translational infrastructure to develop and translate a suite of optical technologies for in vivo diagnosis. This includes the development of optical smartprobes targeting the tumour microenvironment (such as Fibroblast Activation Protein), a FLIM system capable of real-time video-rate FLIM imaging through specialised fibres, which integrate seamlessly with bronchoscopy and robotic navigation systems. Together, this provides a powerful imaging platform, enables access to the smallest lesions where accurate and comprehensive FLIM characterisation could allow immediate diagnosis. This empowers instant initiation of treatments like ablation, creating a new paradigm of see-diagnose-treat for early suspected lung cancer.

The preclinical evaluation of smartprobe development, and FLIM technology development/assessment in lung cancer will be presented as well as some early in vivo data.

Multimodal nonlinear Raman microscopy and endoscopy for cancer diagnostics

Tobias Meyer-Zedler - Leibniz-Institute of Photonic Technology, Jena, Germany

Early detection of disease is of highest importance to fight increasing incidences of cancer in ageing societies. Different multimodal implementations of coherent Raman imaging provide insight into molecular changes at the onset of disease and are due to their label-free nature specifically well suited for routine screening applications and non-targeted analytics. The combination of coherent Raman scattering, two photon excited fluorescence and second harmonic generation imaging for analyzing the composition of tissue composition enables detection of disease induced alterations at an early stage. In this contribution, potential medical applications are presented, i.e., frozen section analysis and endoscopy for routine screening. Compact and powerful mobile multimodal nonlinear imaging platforms are readily realized for label-free hisopathology of native tissue sections, providing great potential for pathologic applications, particularly in combination with AI, i.e., for digital staining. For in

vivo applications, endoscopic imaging devices have been designed, which not only enable visualization, but can also be combined with fs-laser ablation for tissue resection. To further improve the diagnostic potential of the methodology, a broader spectral coverage enables the parallel identification of disease specific marker molecules or compositional changes, which is better suited for complex diagnostic tasks, e.g., tumor margin detection, grading and staging of tumors. Broadband CARS (BCARS) enables the acquisition of the full vibrational spectrum within time frames as short as an individual laser pulse for fast composition diagnostics.

Acknowledgements:

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APPLICATIONS/AI-DRIVEN BIOPHOTONICS – ENVIRONMENTAL MONITORING

6 March // 4 - 5:30 p.m. // Ernst-Abbe Hall

Chair: Dana Cialla-May

Water and Technology – how do they match?

Michael Stelter - Friedrich Schiller University, Jena, Germany

A stable, sufficient and reliable supply of fresh and clean water is a basic human right and a UN Sustainable Development Goal. But this resource is becoming scarce. Climate change puts pressure on water supply for agricultural use, while at the same time the human population is rising and people are more and more concentrated in large cities. Energy supply is limited by the amount of water available, e.g. looking at hydrogen production. The water – food – energy – Nexus is visible more than ever.

On the other hand, technology can help to mitigate risks around water. Starting with sensors, natural and human made water systems, such as rivers, lakes, groundwater reservoirs, freshwater and wastewater systems, can be better understood. Water levels, water quality, pollution and other parameters can be measured digitally and in real time, leading to better water management. Sensors can enable predictive modeling of water systems, leading to more resilience and stability in water supply and treatment infrastructures as well as in aquatic ecosystems. Several photonic sensor principles are currently evaluated for evaluating pollutants in water, for their ease of use, long-term-stability and general robustness.

Once pollution levels and the chemical nature of pollutants are known, technology can also be used to remove these anthropogenic substances from water. Especially in the field of organic micropollutants, such as pharmaceuticals, herbicides or industrial chemicals, photonic water treatment technologies play a critical role. Often applied as photocatalytic reactors, and in combination with other so-called “advanced oxidation processes” (AOP), photonic technologies provide an effective and energy efficient way to destroy organic micropollutants in drinking water and wastewater.

The Thuringian Water Innovation Cluster (ThWIC) is a very large research approach to ad-

dress all these sensor and treatment technologies and combine them with data science and sociological approaches. It's ultimate goal is to contribute to a better global water supply, to the protection of natural water resources and to make water technologies affordable for everybody.

The interplay of spontaneous and stimulated Raman spectroscopy, high-resolution microscopies and the use of machine learning methods in the assessment of the impact of micro- & nanoplastics on human / animal health

Silke Christiansen - Fraunhofer Institute for Ceramic Technology and Systems, Forchheim, Germany

The driving force behind this research stems from the growing occurrence of harmful health effects like various sorts of cancer and kidney diseases in both humans and animal models and the potential role of micro- and nanoplastic particles (MNPs). These effects are now affecting younger individuals more frequently. Additionally, the increasing environmental concerns related to microplastic particles and endocrine-disrupting chemicals (EDCs) add to the urgency of investigating their potential role in the development and advancement of the aforementioned diseases. To delve into this subject, we align spontaneous and stimulated Raman spectroscopy with high resolution microscopies (with light, electrons, ions) and their analytics with the help of the nanoGPSR technology 1,2 that permits data overlay with nanoscale precision. Together with the use of machine learning algorithms for a quantitative assessment of plastic particles and their cell uptake, existing knowledge gaps will be bridged.

The specific use of mouse models provides a nuanced approach to understanding the intricate dynamics between disease progression and plastics particle presence and the details of the particle size, shape, chemical composition, etc.

The use of the aforementioned innovative analytical technologies in their interplay is crucial to ultimately promote a translation of novel findings into clinically relevant procedures / therapies.

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Ultrasensitive and Continuous Monitoring Biosensors based on Plasmon-enhanced Fluorescence

Jakub Dostalek - Czech Academy of Sciences, Prague / Danube Private University, Wiener Neustadt , Austria

Metallic nanostructures allow for the excitation of surface plasmon modes originating from coupled oscillations of charge density that is associated with tightly confined electromagnetic field. These materials increasingly serve in optical sensors and biosensors offering the advantage of probong the sensor surface with enhanced electromagnetic field intensity and local density of optical state. Among others, plasmonic nanostructures find their applications in bioassays relying on plasmon-enhanced fluorescence (PEF) readout method. This approach benefits from strongly increasing brightness of fluorophore molecules (up to a factor > 103) that can be used as labels in numerous formats of sensitive bioassays developed for the analysis chemical and biological species.

This paper will delve on the implementation of ultrasensitive detection scheme for relying on PEF combined with catalytic hairpin assembly – based amplification. Single molecule (digital) detection format is achieved with the help of optimized flexible polymer linker for anchoring of biomolecular recognition elements and rapid enzyme-free cycling reaction, enabling reaching LODs < fM concentrations. The utilization of similar biointerface and PEF optical readout for continuous monitoring of low molecular analytes will be presented and synergies offered between assay formats pursued for the analysis of diseases biomarkers and therapeutic drugs and for the future analysis of harmful compounds relevant to environmental monitoring will be discussed.

Acknowledgements:

This work received support from Operational Programme Johannes Amos Comenius financed by European Structural and Investment Funds and the Czech Ministry of Education, Youth and Sports (Project No. SENDISO - CZ.02.01.01/00/22_008/0004596), and from Technological Agency of the Czech Republic through the project NCK MATCA TN02000069.

Plasmonic refractive index sensing for water quality monitoring: technology and application examples

Christiane Schuster - Fraunhofer-Institute for Ceramic Technologies and Systems IKTS, Dresden, Germany

Miniaturized sensor concepts for cost-efficient and continuous on-site monitoring of the water quality in environmental and agriculture technology, cleantech, food and pharmaceutical industry are as much needed as challenging. For on-site operation, such sensors have to be especially rigid and robust without the need of elaborate sample preparation, which is typically not met by current analytical laboratory methods.

To address these needs, at Fraunhofer IKTS a multiple-use nanoplasmonic sensor was developed for the fast monitoring of micropollutans (in the low µg/L range) and its application demonstrated directly at the effluent of a wastewater treatment plant using the example of diclofenac. A nanostructured gold surface produced by a multi-stage nanoimprint lithography (NIL) process plays a key role in this sensor system and serves as a refractive index-sensitive signal transducer. Subwavelength structuring enables direct excitation of localized surface plasmons (LSPR) in the continuous metal layer with light under normal incidence, resulting in highly efficient, narrowband extinction. The specific binding of a biomolecule near the sensor surface can be observed in the form of a shift of the plasmonic resonance wavelength in the optical transmittance spectrum. In the transmittance setup, optical spectra are automatically recorded with a spectral readout unit at intervals of approx. 1 s and evaluated with regard to their resonance position using an integrated algorithm. To further minimize the optical unit and sensor size, a photocurrent-based evaluation unit was also developed for data acquisition. This uses stacks of two photodiode layers with different spectral sensitivities. The stacked structure enables the detection of changes in the overall spectral distribution by determining the photocurrent ratio of the two wavelength-dependent photocurrents. In the talk, we introduce the sensor unit on the one hand. On the other hand, various application examples are presented: (1) detection of the micropollutant diclofenac at the effluent of a wastewater treatment plant, (2) monitoring of Legionella in drinking water with a mobile unit and (3) analysis of sealice agents in the course of water treatment on board a wellboat.

ABSTRACTS

X. INTERNATIONAL CONFERENCE ON PERSPECTIVES IN VIBRATIONAL SPECTROSCOPY

ICOPVS-SHORT TALKS I

5 March // 9 - 10:30 a.m. // Helene Holzman Room
Chair: Tomáš Cižmár

Holographic CARS endo-microscopy through multimode fibre

INVITED SPEAKER ***Tomáš Cižmár – Leibniz Institute of Photonic Technology, Jena, Germany***

Plasmonic substrates for bioanalytical applications of label-free surface-enhanced Raman scattering

INVITED SPEAKER ***Janina Kneipp – Humboldt University Berlin, Berlin, Germany***

Applications of surface enhanced Raman scattering (SERS) rely on the interaction of plasmonic nanostructures with a respective sample. Probing microstructured bioorganic samples and mixtures of different molecules, such as live cells or biofluids comes with specific challenges, since the accessibility as well as the stability of metal nanostructures used as SERS substrates must be assured. As examples, while SERS of intracellular compartments such as the nucleus of cells, requires the incorporation, and control, of plasmonic substrates in cells,[1,2] the plasma membrane can be brought easily into the proximity of plasmonic nanostructures.[3] In a mixture of molecules, e.g., in body fluids, detection of interesting species, such as products or substrates of specific enzymes may be hindered by co-adsorption of constituents of their matrix. Here, selectivity can be generated by functionalization of the substrate or by electrochemistry-aided interaction.[4,5] We will discuss SERS substrates for bioprobing that can provide a selected interaction with analyte molecules in complex biosamples.

Funding by the Alexander von Humboldt Foundation, EXC 2008 – 390540038 – UniSysCat, and DFG GSC 1013 SALSA is gratefully acknowledged.

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Optical device for combined plasmon and photonic nanojet Raman imaging enhancement

Mile Ivanda - Ruđer Bošković Institute, Center of Excellence for Advanced Materials and Sensing Devices, Zagreb, Croatia

Raman spectroscopy is indispensable method for substance identification and characterization in numerous scientific, industrial and control facilities across many different fields. However, due to the inherently weak signal of Raman scattering, different methods of enhancement have been developed through the years. The most popular and efficient methods today rely on plasmonic enhancement of the collectively oscillating electrons. The examples are surface-enhanced Raman scattering (SERS) and tip enhanced Raman scattering (TERS). However, SERS method has problems with reproducibility and TERS is expensive and complex. On the other hand, photonic nanojet, which is an emerging method gaining popularity, is reproducible, simple and cheap, but it does not achieve such levels of enhancement as plasmonic methods.

Here we present a new optical device which combines plasmonic enhancement with photonic nanojet. The device is called nano-engineered microsphere (NMS) and consists of mechanically controlled dielectric microsphere which has metallic nanoelement built in its shadow side. The microsphere can be of any material and size which is able to generate a photonic nanojet. Numerical simulations are performed which show the generation of the photonic nanojet on the shadow side of the microsphere which then excites plasmons at the tip of the silver nanoelement. Different configurations are simulated where microsphere size, nanoelement size and nanoelement geometry (cone, spike, wire) are varied.

NMS aims to achieve high levels of enhancement and resolution as plasmonic enhancement but retaining reproducibility, simplicity and cheap price of photonic nanojet. Due to the mechanical control of the device and extreme localization of the plasmonic hotspot, it is designed to perform Raman imaging at extremely high resolution. Moreover, the photonic nanojet contribution adds additional enhancement while the microsphere facilitates the scattered light collection. The device with such high potential could be the game changing enhancement method in the future and open new fronts for future research.

Excitation and collection contributions in microsphere assisted Raman spectroscopy

Vlatko Gašparić - Ruđer Bošković Institute, Center of Excellence for Advanced Materials and Sensing Devices, Croatia

The need for efficient substance characterization and rapid growth of technology has brought great achievements in enhancement methods for Raman spectroscopy. One of the newest methods which acquired substantial attention from the scientific community is based on a microsphere generated photonic nanojet (PNJ), which has shown to be a simple, efficient and reproducible method for Raman enhancement.

While the number of scientific publications about PNJ is quickly rising, the mechanism upon which this method works is still unclear. Here we present our research on two contributions to the enhancement: excitational contribution by the PNJ, and collection contribution by the microsphere. The enhancement is experimentally measured on Raman spectroscope by comparing the Raman intensity of the silicon band with and without the microsphere. Different experimental configurations are analyzed where microspheres and microscope objectives are varied. The excitational contribution is investigated by comparing the experimental data with calculations based on Generalized Lorenz-Mie theory of different PNJs. The collection contribution is investigated by comparing the experimental data with our effective numerical aperture model. Additionally, Raman imaging of structured silicon is performed with mechanically controlled microsphere.

The results show a significant collection contribution to the enhancement, along with the expected contribution from the PNJ. The model shows that the microsphere increases the total numerical aperture of the collection system, depending on the microscope objective. By highlighting the so far neglected collection contribution to the enhancement, these findings are of great significance for understanding the mechanism of enhancement and open new pathways for future research.

ICOPVS-SHORT TALKS II

5 March // 9 - 10:30 a.m. // Anna Auerbach Room
Chair: Chandrabhas Narayana

Raman spectroscopy: An emerging tool for drug-protein interactions, protein structure-function, and diagnostic applications

INVITED SPEAKER ***Chandrabhas Narayana - Rajiv Gandhi Centre for Biotechnology, Thycaud P.O., Thiruvananthapuram , India; Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur P.O., Bangalore, India***

The talk is to elucidate the use of Raman spectroscopy in the biotechnology sphere. Raman spectroscopy is a powerful tool in the study of biological samples, especially because it doesn't require extensive sample preparation and looks at the sample in its biologically viable state. This is a growing field in Biotechnology and there is a spurt of papers in this area, mostly from foreign countries. The talk will provide insights into the use of Raman spectroscopy and MD Simulations to study protein structure-function. Since biological samples are in very low concentrations, we use gold and silver nanoparticles to enhance the signals from the biological samples also called Surface Enhanced Raman Spectroscopy (SERS). In addition to this, we also look at understanding the aggregation of proteins like lysozyme which are important for therapeutic applications. In addition, the talk will also provide the ability of Raman spectroscopy to be used in diagnostic applications, like single nucleotide polymorphism (SNP) in plant DNA. For further information see the references below.

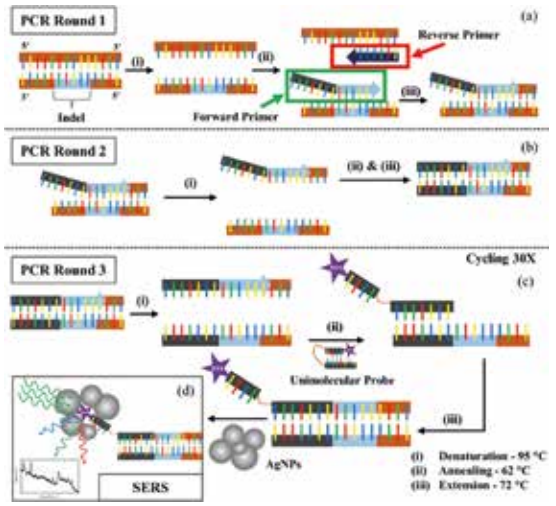

Fig. 1 Schematic representation of the PCR-based SERS strategy. (a) Annealing of mutation-specific FP and RP, with the non-complementary tail of the FP failing to anneal. (b) Formation of the unique, complementary region of the hanging tail. (c) SERS probe binds to its target, the complementary region of the tail. (d) Increased Raman signal from the exposed dye-tagged region of the SERS probe.

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Perspectives of optical photothermal infrared microscopy combined with Raman spectroscopy and fluorescence

Christoph Krafft - Leibniz Institute of Photonic Technology, Leibniz Center for Photonics in Infection Research, Jena, Germany

Optical photothermal infrared (OPTIR) spectroscopy is a vibrational spectroscopic method based on excitation by a pulsed infrared quantum cascade laser, induction of a photothermal effect after infrared absorption and its detection by visible light sources. The principle of visible light detection offers submicron lateral resolution and improved penetration in aqueous buffers. Furthermore, OPTIR can be combined as a correlative approach with other optical modalities such as Raman spectroscopy and fluorescence microscopy. The optical layout is shown in figure 1. The opportunities of the commercial OPTIR instrument Mirage (Photothermal Inc, USA) are demonstrated for microplastic detection, screening of single cells in aqueous buffer, and assessment of tissue sections.

The detection of microplastic particles below 20 µm diameter by direct infrared spectroscopy (e.g. Fourier transform infrared) is impaired by Mie scattering, fringes and dispersion effects. The detection of microplastic particles by Raman spectroscopy can be complicated by resonance enhanced signals of pigments and/or fluorescence background. The simultaneous acquisition of IR and Raman spectra from microplastic particles was shown to give more reliable identification [1].

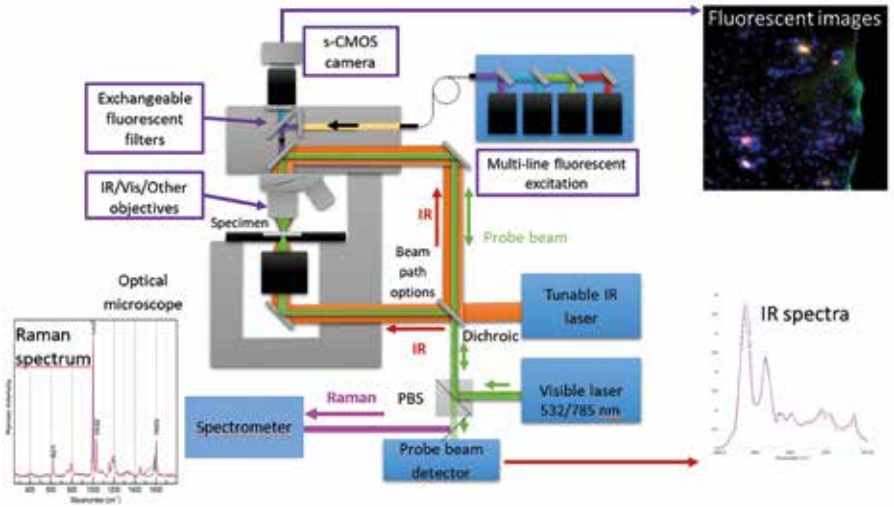

Figure 1: Optical layout of an optical photothermal infrared instrument with Raman and fluorescence modalities for correlative microscopy.

IR studies of single cells in aqueous buffer suffer from strong IR absorption of water and lateral resolution near 10 µm. Due to the relatively large heat capacity of water, the OPTIR spectra of cells in aqueous buffer are less affected by overlapping water bands. 8000 OPTIR spectra of ca. 1600 cells were collected and classification models were trained to classify six cell types. Distinctive IR spectral variations correlated with subcellular features in OPTIR images. The combination of spectral and lateral information can be exploited in the future to improve classification by deep learning frameworks.

The throughput of cell screening by OPTIR can be accelerated by fast scanning. The resulting lower signal-to-noise spectra and images can be subjected to denoising workflows that are also based on neural networks. This concept has already been shown for Raman spectroscopy [3] and offers further perspectives for OPTIR spectroscopy and imaging.

Acknowledgments

This work is supported by BMBF, funding program Photonics Research Germany (13N15464) and is integrated into the Leibniz Center for Photonics in Infection Research (LPI).

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Label-free infrared-vibrational flow cytometry

Marinus Huber - Leibniz Institute of Photonic Technology, Jena, Germany / Max Planck Institute of Quantum Optics, Garching, Germany / Ludwig Maximilians University Munich, Garching, Germany

Flow cytometry is a powerful tool for studying single cells and particles in large quantities, providing crucial biological and medical insights. Its remarkable capacity to extract biologically relevant information quickly and efficiently relies primarily on the integration of fluorescent labels - an approach that is both sensitive and selective, although it relies on targeting and lacks label-free properties. Despite the progress made, label-free methods are in demand. This need stems from the limitations of fluorescent labels, as they are not always available, can be potentially toxic and may incur significant costs. As these problems persist, various efforts have been made to explore label-free alternatives. In this context, vibrational spectroscopy is a particularly promising candidate [1,2], since it combines the advantages of minimum sample preparation, non-destructive, label-free acquisition of the chemically-specific signal, and the potential of ultra-short acquisition times. The use of infrared (IR) spectroscopy for such applications has so far been precluded by the strong IR absorption of liquid water in the context of the low brilliance of contemporary radiation sources. Recently, field-resolved spectroscopy (FRS) [3] employing brilliant, waveform-controlled femtosecond-laser-based IR sources, along with field-sensitive detection now approaching ultimate sensitivity [4], has revealed a route toward overcoming these limitations. Here, we present first high-speed IR measurements of particles in flow.

A field-resolved spectrometer with rapid spectral acquisition at 38 kHz [5] is used to investigate individual particles and cells in flow (Fig. 1a). Broadband, waveform-stable IR pulses with 70 mW of average power are focused to a 40-µm spot (1/e2-intensity diameter) onto an infrared-transparent microfluidic chip. A stream of particles suspended in buffer is hydrodynamically focused, continuously transporting particles through the IR focus, and corresponding spectra are recorded in less than 1 ms (Fig. 1b).

With a throughput of up to 100 particles per second, we collected more than 25000 spectra from individual PMMA and PS particles at different diameter, as well as from yeast and THP-1 cells. Combining density-based spatial clustering with t-distributed stochastic neighbor embedding, reveals that all measured particle types could be separated from each other (Fig. 1c). Due to the size-dependent Mie effect, particles of the same type but of different sizes can also be distinguished.

These findings showcase the potential of field-resolved spectroscopy in realizing infra-

red-based, label-free flow cytometry and sorting of human cells for the first time. Already, different particle types can be identified at the individual level by their vibrational spectra with acquisition times as short as 1 ms. Future applications will benefit from the wider bandwidth and sensitivity of next-generation spectrometers, simultaneously increasing the amount of molecular information obtained and the throughput. This technique could significantly expand the scope of vibrational fingerprinting of biological systems and enable high-throughput screening for low-abundance circulating tumor cells [1].

Acknowledgments

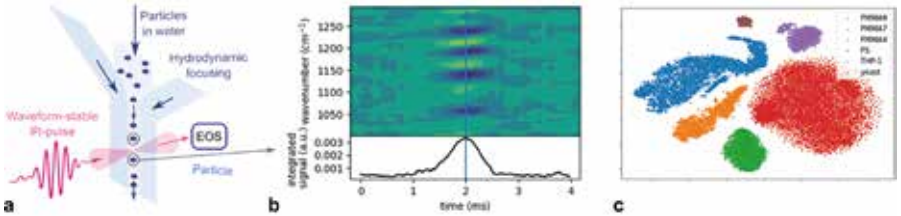

Figure 1: a) Schematic of the channel geometry transporting particles through the IR focus. b) Spectral change over time for a typical event. c) Cluster analysis of more than 25000 spectra from individual particles.

Financial support is gratefully acknowledged: BMBF in the framework of the project SARSCoV2Dx (13N15742); Leibniz Center for Photonics in Infection Research; German Research Foundation under Germany's Excellence Strategy-EXC 2051-Project-ID 390713860; Max Planck Institute of Quantum Optics; Max Planck Technology Transfer program; Centre for Advanced Laser Applications

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Investigating labeled ceramide in living cells using surface enhanced Raman scattering

Yiqing Feng - Humboldt-Universität zu Berlin, Berlin, Germany; Technical University Berlin, Berlin, Germany

Ceramide, the simplest sphingolipid, acts as important structural component and regulator of biological function. The potential of surface-enhanced Raman scattering (SERS) as local vibrational probe of lipid-nanostructure interaction in lipid bilayers has been reported in molecular models containing ceramide and other sphingolipids1,2. Labeled by the fluorescent dye NBD (4-Chlor-7-nitrobenzo-2-oxa-1,3-diazol), ceramide can be employed to follow sphingolipid metabolism and localize Golgi apparatus, membranes and vesicles3.

Here, we studied NBD-ceramide and NBD in molecular and cellular models using SERS, to explore the capacity of SERS to follow cellular changes after the uptake of NBD-ceramide or NBD in living cells. SERS spectra of NBD-ceramide and NBD with gold nanoparticles were obtained, and bands were assigned. We then treated fibroblast and macrophage cells of cell lines 3T3 and J774, respectively, with NBD-ceramide and NBD separately after the incubation with gold nanoparticles. As will be discussed, the statistical analysis of SERS spectra from live cells reveal common features related to the interactions of protein and gold nanoparticles, while there are also spectral differences indicating diverse interactions of intracellular components and gold nanoparticles with different incubation schemes. Moreover, we discuss the distinct spectral features that were observed between 3T3 and J774 cells with the same incubation conditions.

The results demonstrate the potential of SERS with gold nanoparticles to probe the intracellular physiological processing of labeled ceramide in cells and will benefit to study ceramide without labels and further the enzyme function in lipid metabolism in cellular models and other systems.

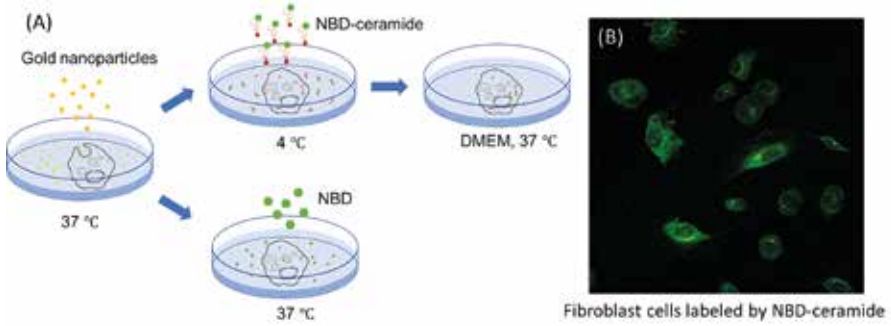

Figure 1: (A) Scheme of cell samples incubated with gold nanoparticles, NBD-ceramide and NBD for SERS experiments, and (B) fluorescence image of fibroblast 3T3 cells incubated with NBD-ceramide.

We thank the support from EC2/BIG-NSE and Germany's Excellence Strategy – EXC 2008 – 390540038 – UniSysCat.

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Investigations of photocatalytic gas conversion using ultrabroadband fs-CARS

Tom Lippoldt - Friedrich Schiller University, Jena, Germany

Photocatalysis is a possible way to reduce CO_2 by conversion to higher value fuels. However, there is a lack of in-situ diagnostic techniques for a better understanding of these processes, for example to characterize transient states. In the present study, we use ultrabroadband coherent anti-stokes Raman spectroscopy (CARS) to investigate reduction reactions of CO_2. Ultrabroadband CARS is used as a modern method to evaluate the concentration of all gases inside the reaction volume. Here, a sufficiently broad laser pulse provides the pump frequency ω_L as well as the Stokes frequency ω_S simultaneously. Thus, the pump/Stokes process is performed in a singular laser pulse.

CO_2-methanation is one possible chemical reaction which can oxidize CO_2 into fuels. In this case, CH_4 is the target product, as it is widely used in the chemical industry. The reaction equation is given by CO_2+4 H_2⇌CH_4+2 H_2O. Rh/Al_2O_3 nanoparticle photocatalysts are known to accelerate this reaction and to favor it over other possible reaction paths with identical feedstock materials.[1]

The CARS setup is powered by a dual-output OPCPA ultrabroadband ultrashort laser source (venteon OPCPA, Laser Quantum GmbH) featuring 10 µJ, 7 fs, 200 kHz.[2] Due to the broad spectrum (Figure 1(a)) Raman transitions of up to 4200 cm^{-1} can be excited. For the probe pulse the secondary output of the laser is generating a 0.7-2 ps laser pulse at 517 nm. All beams are collinearly focused into a reaction gas cell (f=100 mm). The CARS signals are detected in transmission by a spectrograph (Shamrock 500i). An automated delay line is used to control the temporal difference between pump/Stokes and probe pulse, which allows the separation of resonant and nonresonant CARS signals. Rh/Al_2O_3 nanoparticle photocatalysts were used to observe the CO_2-methanation reaction inside the cell. Since the absorption region of the catalyst is mainly in the UV region[3], a Hg-Lamp is used as illumination source (Figure 1(b)). For all measurements, the reaction cell is heated to 400 °C. The reactants have a composition of 20 % CO_2 and 80 % H_2 at 5.0 bar.

CO_2, H_2 and CH_4 show significant CARS signals (Figure 2(a)), when the laser focus is directly above the catalyst. For CH_4, the observation over a reaction time of 60 minutes is shown in Figure 2(b). A steady increase for the CH_4 signal can be seen. This indicates a steady reaction being driven inside the reaction cell. This behavior is confirmed by measurements with a conventional gas chromatograph.

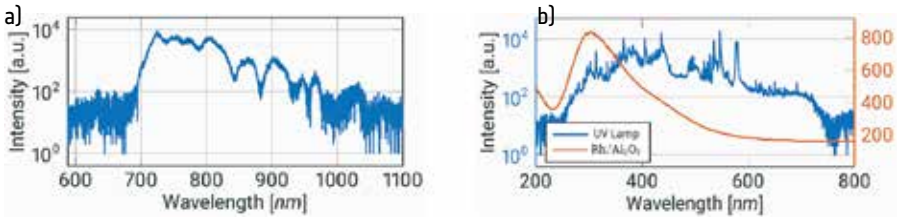

Figure 1 (a) Spectrum of the ultrabroadband ultrashort laser. (b) Spectrum of the UV-Lamp and a diffuse reflection spectrum of Rh/Al2O3.[3]

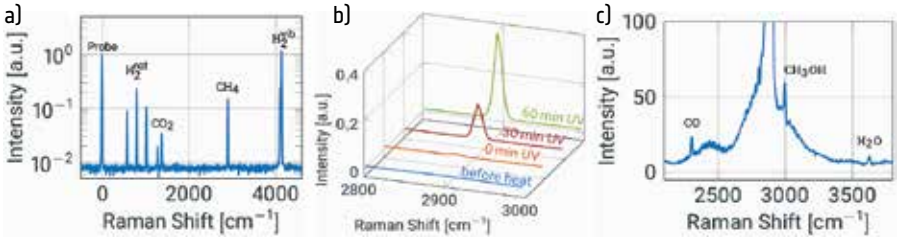

Figure 2 (a) Normalized CARS spectrum of the gas mix during reaction. (b) CH_4 CARS signal of the gas mixture at different time stops of the reaction. (c) CH_4 peak region after 120 minutes reaction time with CARS signals of reaction intermediates and byproducts.

After a reaction time of 120 minutes, besides the predicted signals for CO_2, H_2 and CH_4, additional lines appear at 2306, 2996 and 3626 cm^{-1}. These lines can be attributed towards CO, CH_3 OH and H_2O respectively. This shows that potential reaction byproducts and intermediates are detectable, enabling further investigations of the catalytic dynamics.

The proof of principle experiment demonstrates that ultrabroadband, two-beam CARS is suitable for in-situ investigations of photocatalysis. In the current configuration CH_4 is detected as the main reaction product. Additionally, the observation of reaction byproducts and intermediates CO and CH_3OH allow for future insights of catalytic reaction kinetics.

Acknowledgments

We thank Dr. Izabela Firkowska-Boden for the synthesis of the Rh/Al_2O_3 catalysts.

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ICOPVS-SHORT TALKS III

5 March // 11 a.m. - 12:30 p.m. // Helene Holzman Room
Chair: Giulietta Smulevich

Heme biosynthesis in Gram-positive bacteria

INVITED SPEAKER ***Giulietta Smulevich - University of Florence, Sesto Fiorentino (FI), Italy***

In 2015 it was discovered that monoderm bacteria produce heme b using a different biosynthetic pathway than humans [1]. In detail, coproporphyrin ferrochelatase (CpfC) incorporates ferrous iron into coproporphyrin III (cpIII) to give ferric coproheme, which is eventually decarboxylated to yield heme b by the coproheme decarboxylase (ChdC) enzyme in the final step of this biosynthetic process. This seminar will focus on the spectroscopic study of heme biosynthesis in antibiotic resistant Gram-positive bacteria of the Firmicutes and Actinomyces phyla. Recent insights into the mechanisms of iron incorporation into cpIII by CpfC and on the stepwise decarboxylation of coproheme will be presented [2-4]. The results provide significant and new intriguing information on the catalytic reaction pathway. The understanding of the structure-function correlation of enzymatic mechanisms in heme biosynthesis is essential for the development of new therapeutic strategies.

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Unraveling the Secrets of Cellular Metabolism: A Journey into the World of Inflammation and Activation

Aleksandra Borek-Dorosz - Jagiellonian University, Krakow, Poland

Our body is similar to a musical orchestra, where each section can be attributed to different systems in the human body. The advancement of civilization has led to changes in environmental conditions that can impact how our body works, resulting in various disorders that

could be linked to diseases specific to a civilization. The development of these diseases is commonly correlated with either inflammation or the activation process of cells. The ability to track metabolic, phenotypic, or morphological changes during inflammatory or activation processes may be used to understand better the development of these disorders and new treatment strategies. Such possibilities offer molecular imaging using Raman spectroscopy and spontaneous and modern nonlinear techniques such as Stimulated Raman Spectroscopy (SRS).

Endothelial cells (ECs) are the single cell layer that lines the blood and lymphatic vessels. Since the EC is the first line of defense against inflammation in the cardiovascular system, its dysfunction can lead to the development of cardiovascular diseases [1]. Endothelial metabolism depends on the availability of energy substrates, which involve four major metabolic pathways, of which glycolysis is the most significant [2]. The metabolism and glucose uptake may reflect the physiopathological conditions and cell activity correlated with energy metabolism. Two glucose analogs - d7-glucose and 3-O-propargyl-D-glucose (3-OPG)- were used to study changes in glucose uptake at the subcellular level. 3-OPG allows us to follow its uptake by tracking the characteristic Raman band at 2124 cm-1. What is more, for d7-glucose, the metabolism of glucose was possible to track due to the occurrence of the 1602 cm-1 band. This band was previously called the Raman spectroscopic signature of life, but we hypothesized that this band is not directly related to mitochondrial activity but to cellular metabolism.

The high glucose (HG) state in ECs was induced by the incubation of ECs with 30 mM of d7-glucose or 3-OPG in a glucose-free medium, while the inflammation of ECs was caused by pre-treatment with tumor necrosis factor-alpha (TNF-α). Changes in the metabolism in normal cells and inflamed ECs exposed to HG were investigated utilizing spontaneous and stimulated Raman scattering microscopies. The results show that normal ECs cultured in a glucose-free medium can change their metabolism to fatty acids by excluding glucose from the culture medium. The inflammatory state acts differently on glucose uptake for two studied analogs; for d7-glucose, it enhances its uptake, while in the case of 3-OPG, uptake decreases. In the case of d7-glucose, metabolic changes were also correlated with a substantial increase in the ratio of lipid/protein bands and an increase in the level of lipid unsaturation. Furthermore, an increased cytochrome signal from the perinuclear area indicates accelerated mitochondrial activity.

Activating white blood cells, known as leukocytes, is a crucial step in the inflammation process. Depending on the type of leukocyte, there can be various molecular responses during inflammatory conditions. T cells, a vital immune system component, play a central role in the adaptive immune response. T cells are developed from hematopoietic stem cells through lymphopoiesis [3]. However, for them to become fully functional effector cells, they require activation. This activation is triggered by extracellular stimulatory signals, mainly mediated by a complex of integral membrane proteins called T cell receptor (TCR) complexes. These complexes participate in the response to an antigen. T cell activation involves a series of biochemical intracellular events leading to the production of subtype-specific effector proteins and accelerated proliferation [4]. In our studies, we applied label-free spontaneous Raman imaging and SRS methods to characterize and discriminate activated states in T cells. We have successfully defined spectral biomarkers which can be used as efficient, rapid, and label-free approach to differentiate between normal and activated T cells.

This work was supported by „Label-free and rapid optical imaging, detection and sorting of leukemia cells" project, which is carried out within the Team-Net programme (POIR.04.04.00-00-16ED/18-00) of the Foundation for Polish Science co-financed by the European Union under the European Regional Development Fund and by a grant from the National Science Centre Poland (NCN) (OPUS15 no. DEC-2018/29/B/ST4/00335 to MB).

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Advancing Raman Spectroscopy in Combination with Multimodal Instrumentation for In Vivo Diagnostics and Cellular Analysis

Iwan W. Schie - University of Applied Sciences Jena, Germany; Leibniz Institute of Photonic Technology, Jena, Germany

Raman spectroscopy offers label-free and non-invasive molecular information from biological samples, showcasing vast potential for diagnostic applications. In biomedical applications, Raman spectroscopy (RS) is primarily utilized in two areas: fiber-optic-based systems for clinical in vivo endoscopy and microscopy-based systems for cell characterization. In recent years, we have intensively focused on both areas, developing endoscopy systems for use in various in vivo studies, including those targeting bladder, head, neck cancers, and cardiology. Furthermore, we have enhanced the development of high-throughput Raman spectroscopy (HTS-RS) systems, enabling multimodal and high-throughput analysis of thousands of cells, now employed in diverse clinical studies. This presentation will concentrate on these topics,

addressing the challenges and future perspectives in the field.

The clinical application of RS, however, confronts challenges, including technological limitations in imaging acquisition and regulatory hurdles, such as the new Medical Device Regulation (MDR2017/745) in Europe. Our recent innovations tackle these issues with a Raman-probe based imaging approach that integrates fiber-optic systems for in vivo endoscopy and fiber-optical probes with real-time image processing. This approach allows for the visualization of molecular information on a computer screen or directly on the sample, creating an augmented molecular reality image.

Moreover, we have developed a fully multimodal optical system that integrates phase-contrast, fluorescence, and brightfield microscopy with RS for comprehensive cell characterization. This system augments traditional high throughput systems (HTS) based on fluorescence labeling and imaging microscopy, crucial in biomedical research and drug discovery, with label-free methods like RS. The system opens-up new applications and significantly extends the capabilities of conventional Raman-based cell characterization. This integrative approach facilitates detailed spectral and spatial sample analysis, paving the way for advancements in both research and clinical applications.

Acknowledgments

We acknowledge funding from tthe BMBF (Federal Ministry of Education and Research) and parts of this work are integrated into the Leibniz Center for Photonics in Infection Research (LPI). The LPI initiated by Leibniz-IPHT, Leibniz-HKI, UKJ and FSU Jena is part of the BMBF national roadmap for research infrastructures. European Union's Horizon 2020 research and innovation program under grant agreement no. 667933 (MIB). We also acknowledge the projects EASYprobe - Multimodal, endoscopic, fiber optic probes for clinical imaging diagnostics - new concepts and manufacturing technologies (BMBF, FKZ: 13FH578KX1), PüDE - Promotion über Dreißig (BMBF, 03FHP175); OpenLab-KI - Application of AI and explainable AI for cross-domain processing of OCT-Images (BMBF, FKZ: 16DKWN111), Carl Zeiss Foundation, OptoCarDi – Research and translation of a multimodal optical catheter for the diagnosis of myocarditis, (CZS, grant number P2022-07-003).

Nano-infrared spectroscopic imaging: Promises and Challenges for Application in Biophotonics

Daniela Täuber - Leibniz Institute of Photonic Technology, Jena, Germany; Friedrich-Schiller University Jena, Jena, Germany

Recently, a number of nano IR spectroscopic imaging methods have been developed, overcoming the limitation of long IR wavelengths due to optical resolution by integration of other detection schemes[1], for example the use of visual wavelengths or scanning force microscopy.

The Life Sciences will ultimately benefit from the ability to achieve chemical information at subcellular and single molecule level. High spatial resolution leads to a considerable reduction of the number of chemical bonds contributing to the signal. In Material Sciences, components usually can be easily discriminated by separate IR absorption bands. Yet, in biomaterials, important chemical variations have to be identified above a rather heterogeneous background.

Since 2019 my team BioPOLIM has investigated the advantages and limitations of mid-IR Photo-induced Force Microscopy (PiF-IR). We applied PiF-IR and tapping AFM-IR to a variety of materials ranging from organic monolayers on various substrates and biopolymer compositions[2,3] to single bacteria and human retina which we receive from or collaborators. In collaboration with other groups at the Leibniz-IPHT in Jena, we investigated interference effects in layered systems comparing experimental and calculated FTIR spectra of polymer films on different substrates to PiF-IR spectra and to spectra obtained using optical photothermal IR spectroscopy (OPTIR). We find similar effects in FTIR and OPTIR spectra, while PiF-IR spectra differ from their corresponding FTIR spectra due to the high surface sensitivity of the method[4]. PiF-IR applied to F-Actin prepared from Actin Binding Protein Biochem Kit revealed nanoscale variations in absorption bands @1655 cm-1 and @1630 cm-1 related to α-helices and β-sheets, respectively[5].

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Advancing Skin Cancer Diagnosis: A Novel Multimodal Optical System for Non-invasive Examination of Cutaneous Melanoma

Di Wu - Hannover Centre for Optical Technologies, Leibniz University Hannover, Hanover, Germany

Cutaneous melanoma is one of the deadliest forms of skin cancer, contributing to more than half of the skin cancer-related deaths that have occurred annually over the past several decades. A novel multimodal optical system is proposed for efficient and non-invasive skin cancer diagnosis. The system integrates optical coherence tomography (OCT), ultrasound tomography (US), photoacoustic imaging (OA), and Raman spectroscopy (RS) in a single measurement head, see Figure 1. The combination of these modalities enables a comprehensive and rapid (<2 min) evaluation, providing structural, depth, and chemical composition information as a painless and non-invasive alternative to histological examination.

Melanocytic skin and adjacent areas of normal skin from 30 patients with suspected skin cancer were measured with our system in a clinical setting. The US and OA obtained morphological information of the lesion site, and the lesion infiltration depth matched well with the depth information acquired from subsequent histopathological examination. OCT yielded a high-resolution morphometric map of the superficial surface of the lesion, as well as the precise localization for RS measurements. RS, in turn, provided information on the chemical structure of the lesion, showing a higher lipid content and a significantly lower carotenoid content in melanocytes compared with normal skin. In addition, the background fluorescence intensity of Raman spectra of lesion skin and normal skin was found to be significantly different. By using a support vector machine (SVM), taking the spectral data containing fluorescence as an input an accuracy of 89.1% for the classification of melanocytic skin and normal skin was achieved.

Our results indicate that the proposed multimodal optical imaging system has the potential to diagnose skin cancer in the future. Compared to traditional histopathological detection methods, the proposed system does not require surgical excision of the lesion to confirm the diagnosis, greatly reducing the surgical pain of patients, especially when the lesion is benign. Next, we will look for more cases of melanoma and other types of skin cancer to further advance the approach and potentially achieve non-invasive diagnosis of skin cancer without the need for histopathological surgery.

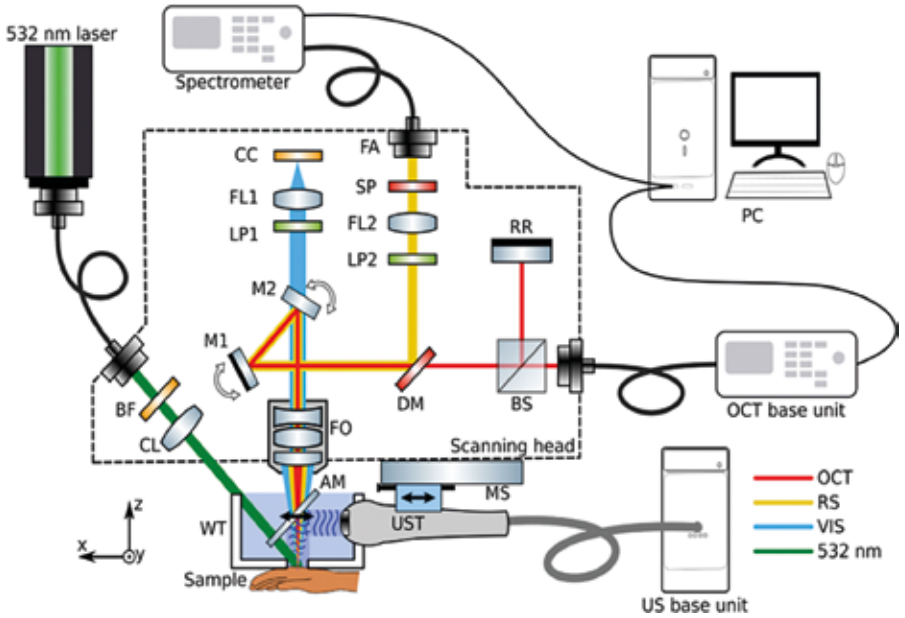

Figure 1: Sketch of the experimental setup. AM, acoustical mirror; BF, bandpass filter; BS, beam splitter, CC, camera chip, CL, collimating lens; DM, dichroic mirror; FA, fiber adapter; FL, focusing lens, FO, focusing objective; LP, long pass filter; M, galvo mirrors; MS, motorized stage; OCT, optical coherence tomography; RR, retroreflextor; SP, shortpass filter, UST, ultrasound transducer; WT, water tank.

Acknowledgments

The authors acknowledge financial support from the German Research Foundation DFG (German Research Foundation, Project ID RO 3471/18-1 and EM 63/13-1). Also, financial support from the German Research Foundation (DFG) under Germany's Excellence Strategy within the Cluster of Excellence PhoenixD (EXC 2122, Project ID 390833453) is acknowledged.

ICOPVS-SHORT TALKS IV

5 March // 11 a.m. - 12:30 p.m. // Anna Auerbach Room
Chair: Thomas Mayerhöfer

Infrared molecular fingerprinting for phenotyping health and disease

Mihaela Žigman - Ludwig Maximilian University of Munich (LMU), Garching, Germany / Max Planck Institute of Quantum Optics (MPQ), Garching, Germany;

Recent advances in optical spectroscopy have unveiled new opportunities for probing living systems at a molecular level. Our primary objective is to advance and assess vibrational spectroscopy as an analytical framework for comprehensive cross-molecular profiling of systemic human biofluids and to evaluate the feasibility of employing infrared fingerprinting for high-throughput in vitro biomedical diagnostics. More specifically, we are investigating its viability for the analysis of human blood serum and plasma within the context of clinical diagnostics.

By combining vibrational fingerprinting of liquid blood plasma and serum with the integration of data analyses using machine learning, the results based of various studies1,2,3,4 will be discussed. On a smaller scale, we have uncovered a remarkable degree of stability in the infrared molecular fingerprints within individuals over time1, laying a crucial foundation for potential health screening applications.

In Lasers4Life study, encompassing several thousands of individuals within case-control settings, we have gathered evidence indicating that the spectral information of plasma and serum contains distinct signatures for four types of cancer2. The effectiveness of disease detection is linked to the stage of cancer progression. We underscore the potential for early cancer diagnostics, highlight possible applications forging primary cancer diagnostics and provide evidence for distinguishing between different cancer entities. Yet, blood-based vibrational fingerprints are not able to detect only very severe health phenotypes like cancer. We have also found that infrared spectra have the capacity to just as well detect common chronic health deviations. Interestingly, in a large-scale population scenario with its inherent heterogeneity, we identified further potential of infrared fingerprinting to distinguish between various co-occurring conditions, opening up the possibility of screening for a variety of conditions and enhancing risk stratification.

The discussion will center around the technological and analytical framework, as well as the potential and limitations of cell-free blood-based infrared molecular fingerprinting - a versatile platform offering multi-phenotyping capabilities and providing insights into explainable healthcare analytics.

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Widefield Super-Resolution IR Imaging with Fluorescence Enhanced Photothermal Infrared

Miriam Unger - Photothermal Spectroscopy Corp GmbH, Duisburg, Germany / Photothermal Spectroscopy Corp, Santa Barbara, USA

Optical Photothermal Infrared (O-PTIR) spectroscopy has established itself as a breakthrough vibrational microspectroscopy tool, offering significant advantages over the traditional FTIR/QCL & Raman spectroscopy, providing submicron simultaneous IR+Raman and fluorescence imaging, in non-contact mode with high sensitivity without any dispersive scattering artefacts.

O-PTIR has generated significant research interest and publications, however there still exists a demand for rapid, high sensitivity and high resolution widefield IR imaging. To this end, we have developed a novel widefield super-resolution IR imaging approach that utilizes the fluorescent signal directly for IR signal extraction. As the fluorescent signal is captured with a 2D fluorescence camera, this generates, simultaneously, widefield IR imaging as well as widefield fluorescence images. We have termed this - Fluorescence-Enhanced Photothermal Infrared (FE-PTIR) spectroscopy.

The key enabling factor here, is that when the wavelength of the IR pulses is tuned to a molecular vibration of fluorescently labeled molecules, the absorbed heat causes a modulation in the amount of fluorescent light emitted from the fluorophores and it's surrounds. Coupled with the parallel data acquisition via the 2D (megapixel) visible fluorescence camera, using a standard glass objective of 50x, 0.8NA, single field of view for IR of 70x70um with 200nm pixels are possible. Compatibility with other standard visible glass objectives such

like those with higher NA, or even immersion objectives opens up further possibilities for widefield super-resolution IR imaging.

FE-PTIR thus allows the IR spectroscopic analysis of specifically labeled regions of biological cells and tissue, for example to study conformational stages of a specifically labeled class of target proteins. FE-PTIR can enable the study protein misfolding associated with neurodegenerative diseases. Various examples from these applications will be provided.

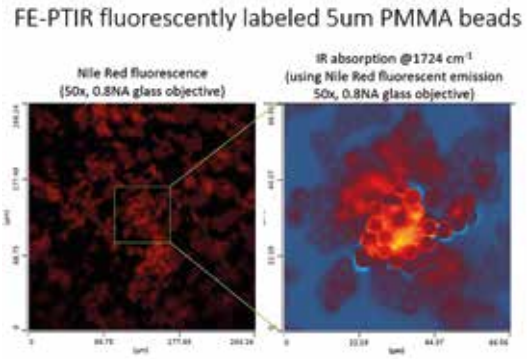

Figure 1: Nile Red labelled 5micron PMMA beads, widefield epi fluorescence image (left), chemical image at 1724cm-1 collected via FE-PTIR

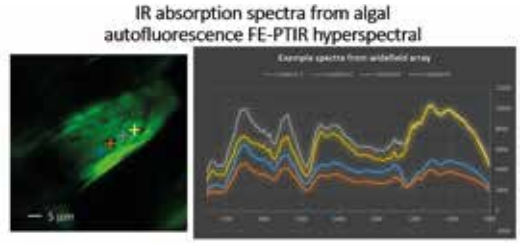

Figure 2: Autofluorescence derived O-PTIR hyperspectral from algal cells. Left, protein (1660cm-1) FE-PTIR imaging and right, spectra reconstructed from market locations on image

How to evaluate effects of antimicrobials on microbial Raman spectra by AI methods

O. Samek - Institute of Scientific Instruments of the Czech Academy of Sciences, Brno, Czech Republic.

The ability to identify and characterize microorganisms (bacteria, eukaryotic cells) from minute sample volumes in a rapid and reliable way is the crucial first step in the classification of microbial infections. Ideally, analytical techniques would require minimal sample preparation, permit automatic analysis of many serial samples, and allow rapid classification of these samples with reference to a stable database. Current practice, however, is far from being ideal, and typical analytical procedures may take several hours to days to complete. Several studies have shown that Raman microspectroscopy is capable of rapid identification and discrimination of biological samples, including medically relevant microorganisms (e.g., bacteria, yeast). This experimental technique employs a laser beam that is focused with a microscope objective in order to excite and collect Raman scattering spectra from a small volume of the sample (<1 femtoliter). A typical Raman spectrum contains a wealth of information indicative of the cellular content of nucleic acids, proteins, carbohydrates, and lipids. Such a spectrum functions as a cellular 'fingerprint' and serves as a sensitive indicator of the physiological state of the cell. Raman spectra thus enable to differentiate cell types, actual physiological states, nutrient conditions, and phenotype changes. In principle, Raman spectroscopy requires measurement times in the order of minutes, and sample preparation can be short and extremely economical. An added advantage is the fact that the cells are still in contact with the culture medium and are kept viable, thus providing a spectroscopic signature of the cells "in-situ".

Objectives: Here we report on the effects of antimicrobial agents on microbial Raman spectra. In this pilot study, we used the Candida albicans ATCC 90028 strain, Staphylococcus aureus ATCC 25923 strain, and Staphylococcus epidermidis ATCC 12228 strain. Both staphylococcal strains were exposed to clindamycin, vancomycin, and ceftaroline; the C. albicans strain was exposed to amphotericin B, caspofungin, and voriconazole.

To assess the effect of antimicrobials on Raman fingerprints of microbes, we compared the spectra of bacteria/yeasts after exposition to subinhibitory concentrations of antimicrobials and non-exposed microbes using the Raman spectrometer (inVia Raman Spectrometer Renishaw plc., Wotton-under-Edge, UK), with 785 nm single-mode diode laser as the excitation source focused on a sample using a microscope (Leica, Wetzlar, Germany, objective 50×).

Results and discussion - the acquired Raman spectra incorporate differences between fingerprints of exposed and non-exposed microbes. In order to find and quantify the most significant features connected to the antimicrobial strain exposure AI methods – namely PCA, 2D cross-correlation, and regression analysis – were applied. Moreover, the relation of identified features and Raman spectrum peaks/bands will enable us to monitor the effectiveness of the antimicrobial treatment. Further, this pilot study shows that the effects of antimicrobial agents are translated into the specific Raman fingerprint and could be a base for detecting antimicrobial resistance in bacteria/yeasts.

Conclusions - Raman spectroscopy is a powerful tool with numerous applications in

microbiology. It can differentiate among microbial species, and it might have the potential to become a reliable diagnostic tool in the future. Moreover, based on our results it appears to be a valuable tool for monitoring the effects of antimicrobial agents, which can aid in detecting antimicrobial resistance in microbes and choosing appropriate treatments for patients.

Acknowledgements

The work was supported by grants MUNI/A/1361/2022 (Grant Agency of Masaryk University) and AZV NU21-05-00341 (Czech Health Research Council).

Broadband coherent Raman platform for stimulated Raman histology

Matteo Negro - Cambridge Raman Imaging Srl, Milan, Italy

Histopathology plays a pivotal role in diagnosing diseases, particularly cancer. Its dependence on spatial cell and tissue arrangements, revealed through early 20th-century staining methods, faces challenges due to subjectivity, varying protocols, and pathologist expertise, resulting in diagnostic inaccuracies. Recognizing histology's critical role in healthcare, efforts to bolster objectivity and precision are gaining momentum.

Stimulated Raman Scattering (SRS) offers sub-cellular spatial resolution and molecular-specific contrast. It enables label-free chemically-specific imaging by detecting the vibrational properties of tissues. Stimulated Raman Histology (SRH) can be used to visualize histopathological features, enabling quantitative evaluation [1,2]. The current approaches, applicable only to fresh-frozen samples, are based on the acquisition of only two Raman peaks at ~ 2845 cm-1 and 2930 cm-1, selected to maximize contrast between nuclei and cytoplasm [3]. A broadband approach, able to obtain chemically-specific information by analyzing the entire Raman spectrum, is desirable in order to extend SRH applicability to formalin-fixed paraffin-embedded (FFPE) samples, enabling the translation into the clinical-diagnostic routine. Here, we report a broadband coherent Raman platform (CRP) designed to exploit the full potential of SRH. It consists of an all-fiber dual wavelength self-synchronized laser and a detection unit based on a compact multichannel lock-in amplifier [4], that ensures state-of the-art SRS performances over the entire CH spectrum (2800-3100 cm-1), parallelizing the detection of up to 38 spectral channels in 1 µs. Our CRP combines a broadband approach for chemometric and multimodal analysis of tissues (Fig. 1a) with artificial intelligence tools, thus allowing virtual H&E staining and tissue segmentation for diagnostic purposes (Fig.1b).

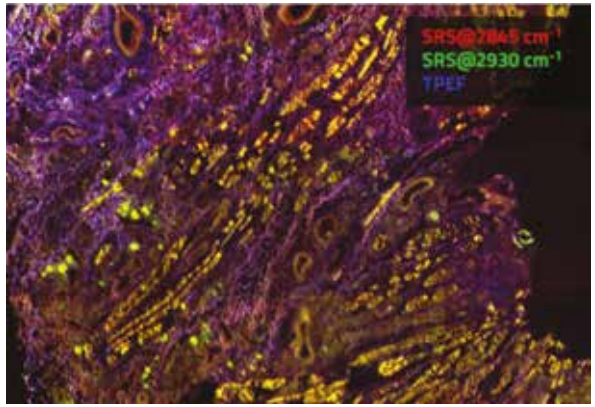

Figure 1: Image of human head and neck tumour tissue obtained combining SRS signal @2845 cm-1 (red), SRS signal @2931 cm-1(green) and two-photon excitation fluorescence (TPEF) signal (blue)

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A screening Test for Alzheimer's Disease Based on Raman Hyperspectroscopy and Machine Learning

Igor. K. Lednev - Department of Chemistry, University at Albany, State University of New York, Albany, USA

Raman hyperspectroscopy combined with advanced statistics is uniquely suitable for characterizing microheterogeneous systems. Understanding the structure and (bio)chemical composition of samples at the microscopic level is important for many practical applications including material science, pharmaceutical industry, etc. We have recently demonstrated a great potential of Raman hyperspectroscopy for disease diagnostics. In this presentation, we will discuss the development of a novel, noninvasive approach for Alzheimer's disease (AD) diagnostics based on Raman spectroscopy of blood, cerebrospinal fluid and saliva. Near infrared (NIR) Raman hyperspectroscopy coupled with machine learning was utilized for differentiating patients diagnosed with Alzheimer's disease, other types of dementia and healthy control subjects with more than 95% sensitivity and specificity. When fully developed, this fast, inexpensive and noninvasive method could be used for screening at risk patient populations for AD development and progression.

Machine Learning Classification of Infrared Spectra from Children with Autism Spectrum Disorder

Filiz Korkmaz - Atilim University, Ankara Türkiye

Autism spectrum disorder (ASD) is a heterogeneous neurodevelopmental disorder caused by multiple factors, lacking clear biological biomarkers. Diagnosing ASD still relies on behavioral and developmental signs and usually requires lengthy observation periods, all of which are demanding for both clinicians and parents. Although many studies have revealed valuable knowledge in this field, no clearly defined, practical, and widely acceptable diagnostic tool exists. In this study, 26 children with ASD, aged 3-5 years, and 26 sex- and age-matched controls are studied to investigate the diagnostic potential of the Attenuated Total Reflectance-Fourier Transform Infrared (ATR-FTIR) spectroscopy. The urine FTIR spectrum results show a downward trend in the 3000-2600/cm region for ASD+ children when compared to the typically developing (TD) children of the same age. The average area of this region is 25% less in ASD+ level 3 children, 29% less in ASD+ level 2 children, and 16% less in ASD+ level 1 children compared to that of the TD children. Artificial urine solutions are used to find the source of the decline in this area. Less-than-normal levels of uric acid, phosphate groups, and/or ammonium can be listed as probable causes. Principal component (PC) analysis was applied to the two groups. The first two PCs account for 93.1% of the total variance within 95% confidence using the entire spectrum window. Lower absorbance in the 3000-2600/cm region of the infrared spectrum, which is the spectral sum of several urine components, correlates with ASD. Support Vector Machine (SVM) and Kernel Neural Network (kNN) were used to establish a classification model. RBF, Linear, and POLY were chosen for SVM, and MINKOWSK and COSINE algorithms were chosen for kNN. Leave-one-out cross validation technique was used. The impact of different spectral pre-processing and the spectral window of choice on the algorithm's classification ability was studied as well. Results were compared in terms of F1-score, accuracy, sensitivity, precision, and Matthews' coefficient. In the sensitivity metric the SVM-poly gave the best results without exception among the various tested conditions. It was found that spectral pre-processing had the greatest impact on the machine learning classification performance rather than the spectral frequency range.

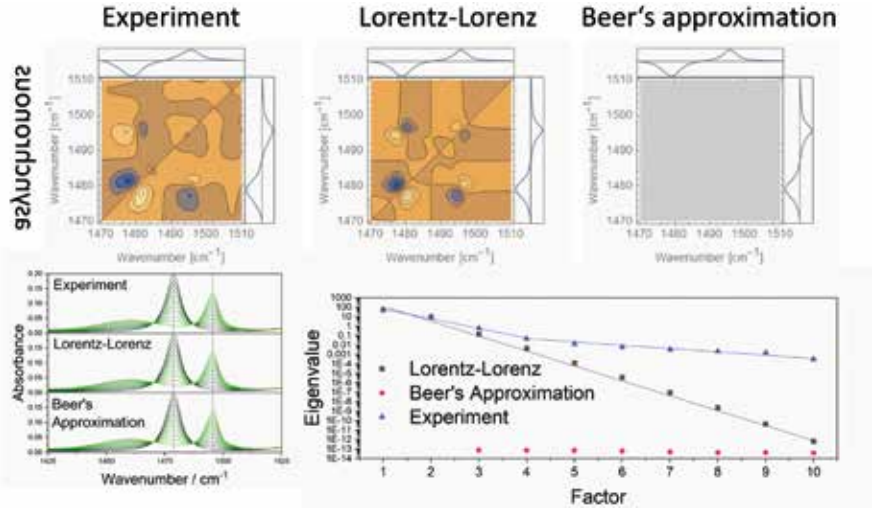
SETTING THE STAGE: LINEAR AND NONLINEAR RELATIONSHIPS IN IR- AND RAMAN-SPECTROSCOPY

5 March // 14 - 15:30 p.m. // Clara and Eduard Rosenthal Room
Chair: Achim Kohler

Are there linear relationships in infrared spectroscopy?

Thomas Mayerhöfer - Leibniz Institute of Photonic Technology, Jena, Germany

In accordance with the Bouguer-Beer-Lambert (BBL) approximation, absorbance exhibits a linear correlation with light path length, molar concentration, and a material constant. Traditional chemometric methods are founded on this approximation. However, when examined from the standpoint of wave optics and dispersion theory, the BBL approximation emerges as a limiting principle applicable to vanishing absorption, neglecting the wave-like



2D Correlation spectroscopy and Principal Component analysis reveal nonlinearities in ideal binary liquid mixtures.

properties of light and its typical nonlinear polarization in condensed matter. We establish this nonlinearity through three illustrative examples. Firstly, we analyze IR spectra of films on index-matched CaF2 substrates with varying thickness. Secondly, we explore IR spectra of ideal binary liquid mixtures concerning their composition. Lastly, we demonstrate that the spectra of micro-heterogeneous mixtures are contingent on the size of the structures. These instances represent just a fraction of the numerous experimental findings that substantiate the intrinsic nonlinearity of the infrared spectral response.[1] Accordingly, it is in general impossible to separate chemical from physical information in IR spectra by analytical methods. Therefore, we think that an application of intrinsically nonlinear methods like neural networks is not only justified, but highly advisable.

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Field manipulation of bands in IR spectra of thin films

Karsten Hinrichs - Leibniz Institute for Analytical Sciences - ISAS, Berlin, Germany

In bio-analytic, materials research and sensing applications it is often a concern to reveal morphological, structural and chemical information from vibrational spectra. For IR spectra of thin films this can be complicated because the observed vibrational band properties depend on the measurement geometry, the film thickness, the materials dielectric functions, and the direction of the probing electromagnetic field. [1] In particular, the absorption and related band properties are manipulated by the electromagnetic field for strong oscillators. This is observed for passivated silicon surfaces, oxide layers but even in unpolarized reflection spectra of an isotropic polymer film or ATR spectra of a polymer bulk sample. This hampers a direct read-out of accurate vibrational band shapes and vibrational frequencies from the measured spectra and optical simulations are required for quantitative interpretation.

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Solvent mediated vibrational coherence decay: Excited state dynamics study using ultrafast Raman loss spectroscopy

Prof. Siva Umapathy - Indian Institute of Science, Bangalore, India

In this talk, we would discuss the influence of solvent dynamics during ultrafast isomerization and proton transfer processes. We have used ultrafast stimulated Raman methodology measuring the Raman loss signals. We have observed that the rate of coherence decay of the exicted state vibrational modes are controlled and mediated by the solvent friction.

A POTPOURRI OF DIFFERENT AI TECHNIQUES APPLIED TO IR- AND RAMAN-SPECTROSCOPY

5 March // 4 - 5:30 p.m. // Clara and Eduard Rosenthal Room
Chair: Siva Umapathy

Pitfalls and challenges in the use of AI-based techniques for vibrational spectral data

Thomas Bocklitz - Leibniz Institute of Photonic Technology, Friedrich-Schiller-University, Jena, Germany

Vibrational spectroscopic techniques likes infrared (IR) and Raman spectroscopy are increasingly used in various disciplines such as chemical analytics, life science and medicine. All these applications need artificial intelligence (AI) based methods to extract high-level information and knowledge from the vibrational spectroscopic data. The high-level information depends on the task and the sample, e.g., disease types, tissue types and other properties of the samples such as concentrations of constituents. To extract this high-level information a specialized data pipeline consisting of experimental design, sample size planning, data pre-treatment, data pre-processing, chemometric and machine learning based data modelling, model transfer methods and transfer learning needs to be constructed. In almost all steps in the data pipeline AI based methods like machine learning and deep learning- can and often must be applied. This talk summarizes pitfalls while utilizing AI-based techniques for vibrational spectral data and highlights the strategies to avoid them, which allows to

Physics- and chemistry-aware data modelling in infrared microspectroscopy

Achim Kohler - Norwegian University of Life Sciences, Ås, Norway

Extended Multiplicative Signal Correction (EMSC) has found extensive application in infrared spectroscopy for effectively modeling intricate scatter and absorption effects. Understanding these effects is crucial as it sheds light on the interaction mechanisms between infrared radiation and matter. Beyond the fundamental insights gained, the practical advantage of such modeling lies in the ability to disentangle absorption and scattering effects in spectra. This separation facilitates the retrieval of pure absorbance spectra, enabling a more precise chemical interpretation of spectral signatures.

Moreover, the removal of scatter signatures from absorbance spectra simplifies the creation of calibration and classification models. This simplification is particularly valuable in cases where training data is limited, and spectral pre-treatment, informed by physics-based a priori knowledge, proves highly beneficial.

The retrieval of pure absorbance spectra from spectra heavily distorted by scattering represents an inverse scatter problem. Essentially, it involves estimating the optical properties of a sample from the measured spectrum. However, inverse scatter problems are inherently ill-posed, given that different optical properties of a particle can yield the same measured spectrum. In this paper, we explore methods to condition the solution space for inverse scatter problems in infrared spectroscopy.

We present and compare three distinct approaches for retrieving pure absorbance spectra in infrared microspectroscopy: (1) EMSC Implementation: Utilizing EMSC with a meta-model derived from Mie formalisms. (2) Neural Network Integration: Employing a neural network trained on EMSC-corrected data and simulated data using the Mie formalism. (3) Hybrid Model: Integrating Mie theory and a neural network into a hybrid model.

Explainable artificial intelligence for infrared and Raman microscopy: A hypothesis-centric perspective

Axel Mosig - Ruhr University Bochum, Bochum, Germany

Deep neural networks have revolutionized the field of biomedical image analysis, including the analysis of infrared and Raman microscopic images. Yet, the black box nature of neural networks constitutes a particular challenge when classifying spatially resolved vibrational spectroscopic images in medical diagnostics or other life science applications: It is generally difficult to assess whether a neural network has identified a molecular or cellular mechanism of disease as the basis for classification, or whether the classification relies on a confounding

information that is present in the training data. Addressing the question of what a neural network has learned is the subject of explainable artificial intelligence, which has become an important discipline in the machine learning field. In this talk, we introduce the framework for falsifiable explanations in artificial intelligence, which puts an experimentally testable hypothesis into the center of establishing deep learning systems. We demonstrate its application in infrared microscopy with applications in detecting and subclassifying cancer in colon tissue as well as localizing and characterizing Aβ-plaques in brain tissue.

APPLICATIONS OF AI-ASSISTED VIBRATIONAL SPECTROSCOPY - CHEMISTRY AND MATERIALS SCIENCE

6 March // 10 - 11:30 a.m. // Siegfried Czapski Room
Chair: Heinz Siesler

Laser-Based mid-IR Dispersion Spectroscopy of Liquids

Bernhard Lendl - TU Wien, Vienna, Austria

When interacting with gaseous or liquid samples, laser radiation does more than attenuate light intensity; it also induces a phase shift in the transmitted light and heats the sample containing the analyte. While direct absorption spectroscopy primarily exploits intensity attenuation, these additional effects form the basis for dispersion spectroscopy and indirect methods like photoacoustic and photothermal spectroscopies.
This presentation will review potential measurement modalities, highlight recent instrumental advancements, and showcase selected applications. For liquid sensing, we employ broadly tunable external cavity quantum cascade lasers. We demonstrate their use in measuring protein secondary structures in water, exemplified by in-line detection in liquid chromatography and protein melting experiments. Dispersion spectroscopy will be introduced through measuring ethanol in water, illustrating its suitability for dynamic reaction monitoring. This will include observing the enzyme-catalyzed hydrolysis of sucrose into glucose and fructose.

Infrared spectroscopic imaging for pathology: from fundamental advances to practical implementation

Rohit Bhargava - University of Illinois Urbana-Champaign, Urbana, USA

Arising from fundamental vibrational modes, IR absorption is the strongest optical signal indicative of molecular composition. In an imaging format, it represents a unique opportunity to understand the chemical composition of tissue and used artificial intelligence (AI)

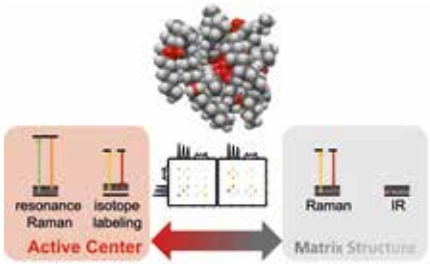
workflows to study disease progression. Unlike optical microscopy for pathology, the need to record a significantly larger quantity of data than a typical microscopy image (MB vs. GB) and the extensive bandwidth of the spectra (~10 um), trade-offs are needed between signal to noise ratio, spatial-spectral coverage, resolution and speed to make practical technology. Here, we present a path from rigorous theory to optomechanical modeling and fabrication that provides new imaging capability. We first describe a new microscope design for increased speed and rapid coverage that is useful for biomedical and clinical tissue imaging. Next, we describe applications that demonstrate the utility of this technology for pathology.

Investigating Active Centers in Complex Matrices with Correlated Vibrational Spectroscopy

Julian Hniopek - Leibniz-Institute of Photonic Technology, Jena, Germany

Many systems of interest in material science gain their functionality by embedding active centers inside matrices. Methods to investigate the molecular structure of these active centers as well as their interaction with the matrix and the environment are therefore crucial for a holistic understanding of such systems.

We have employed Raman- and IR-spectroscopy together with experimental techniques like resonance-enhancement and isotope labeling to investigate a wide range of functional systems, including smart polymers & photocatalysts in situ. Employing analysis techniques to correlate between different spheres of information, especially two-dimensional correlation analysis, it was possible to reveal the molecular mechanisms behind their respective functionalities as well as directly correlate molecular with macroscopic information. Utilizing this vibrational spectroscopy approach with novel analysis methods, allows material scientists to move from a trial-and-error based development approach to targeted synthesis. This can significantly speed up the production of tailored materials, enabling optimal functionality for desired applications.



APPLICATIONS OF AI-ASSISTED VIBRATIONAL SPECTROSCOPY - BIOLOGY AND MEDICINE

6 March // 11 a.m. - 12:30 p.m. // Siegfried Czapski Room
Chair: Igor Lednev

Point-of-care vibrational spectroscopic approaches to parasitic disease diagnosis

Bayden R. Wood - School of Chemistry, Monash University, Clayton, Australia

The prevalence of neglected tropical diseases (NTDs) is advancing at an alarming rate. Malaria and Leishmania's remain a major public health challenge. There is an urgent need for point-of-care diagnostic approaches that are sensitive to low parasitemia, affordable, and easy to use in field settings are urgently required. The presentation will focus on vibrational spectroscopic approach for malaria using portable mid-IR spectrometers and low-cost, miniaturized near-infrared (NIR) spectrophotometer, which was used for the first time to detect and quantify malaria infection in vitro from isolated dried red blood cells. The use of NIR offers several advantages, including wavelength accuracy and repeatability, speed, and resolution, as well as a greatly improved signal-to-noise ratio compared to existing spectroscopic options. Multivariate data analysis was used to discriminate control red blood cells from infected cells, and the technique established the limit of detection. Principal component analysis showed good separation between malaria infected and uninfected RBCs, while partial least-squares regression analysis yielded a robust parasitemia prediction, with a root-mean-square error of prediction values of 0.446 and 0.001% for the higher and lower parasitemia models, respectively. The R2 values of the higher and lower parasitemia models were 0.947 and 0.931, respectively. The estimated parasitemia detection limit was 0.00001%, and a quantification limit of 0.001% was achieved. Further clinical studies with larger patient numbers are required to ascertain the efficacy of the technique for point-of-care screening. Studies will also be presented on Leishmania's parasites within macrophages and also isolated promastigotes using synchrotron FTIR and Raman spectroscopy. This study represents an important step toward the development of a low-cost, easy-to-use, and sensitive diagnostic tool for malaria and Leishmania disease, which could significantly contribute to reducing these cases and related life losses globally by 2030, as per the World Health Organization's objective.

Spectromics facilitate spatial and temporal resolution in regenerative medicine

Julia Marzi - NMI Natural and Medical Sciences Institute at the University of Tübingen, Reutlingen, Germany

Recapitulating cell and tissue dynamics in tissue-engineered constructs that are applied as in vitro test systems or implants can contribute to a better understanding of mechanisms at the cellular interface; ultimately boosting clinical translation. We could demonstrate that time-resolved Raman imaging applied on Organ-on-Chip platforms enabled to monitor cellular dynamics of tumor-immune or host-microbiome interactions at various scales. Data obtained longitudinally or on a large sample size provide comprehensive information that require state-of-the-art analytics to unravel relevant tissue alterations. Therefore, in addition to conventional multivariate methods for spectral processing, algorithms conventionally applied for (spatial) Omics were translated to the analysis of Raman data. The workflow was initially implemented on the tissue scale but could be translated to in vitro models and liquid biopsies. Furthermore, correlative approaches were implemented to enhance the molecular characterization of the samples by integrating multimodal data from additional readouts such as metabolomics, transcriptomics.

Labeled Raman spectroscopy to support metabolomics

Malgorzata Baranska - Jagiellonian University, Krakow, Poland

The use of molecular probes in Raman imaging is a relatively new technique in subcellular research, however, very fast and dynamically developing. Compared to the label-free method, it allows for a more sensitive and selective visualization of organelles within a single cell. Directly visualizing biological structures and activities at the cellular and subcellular levels remains by far one of the most intuitive and powerful ways to study biological problems.
For hyperspectral detection and imaging of living cells, it is very desirable to use probes with strong and unique Raman vibrations in the biological silent region (1800 – 2800 cm^{-1}). Here it is shown a biorthogonal chemical imaging of cells to track biochemical changes associated with mitochondrial function at the cellular level in an in vitro model. Both commercially available and newly synthesized highly sensitive Raman probes for selective imaging of mitochondria in live cells is presented.

APPLICATIONS OF AI-ASSISTED VIBRATIONAL SPECTROSCOPY – PROCESS ANALYTICAL TECHNOLOGY, FORENSIC

6 March // 2 - 3:30 p.m. // Siegfried Czapski Roomi
Chair: Bernhard Lendl

Inherent Intelligence vs. Artificial Intelligence: Curse and Blessing of Infrared Diagnostics

Boris Mizaikoff - Ulm University; Hahn-Schickard, Ulm, Germany

State-of-the-art sensing platforms ideally benefit from miniaturized and integrated optical technologies providing direct access to molecule-specific information. With in-situ sensing strategies in point-of-care diagnostics becoming more prevalent, detection schemes that do not require reagents or labeled constituents facilitate localized on-site analysis close to real-time.
Mid-infrared (MIR; 3-20 µm) photonic platforms/sensing concepts are nowadays increasingly adopted in biodiagnostics capitalizing on the inherent molecular specificity enabling the discrimination of molecular constituents at ppm-ppb concentration levels in condensed and vapor phase media. Recently emerging strategies taking advantage of innovative waveguide technologies such as substrate-integrated hollow waveguides, and planar semiconductor waveguides shaped into sophisticated optical structures (e.g., MIR Mach-Zehnder interferometers) in combination with highly efficient light sources such as tunable quantum cascade and interband cascade lasers (QCLs, ICLs) and interband cascade LEDs (IC-LEDs) facilitate compact yet robust MIR diagnostic platforms for label-free chem/bio sensing and medical diagnostics. The 'inherent intelligence' of the obtained IR spectral information given by the associated 'molecular fingerprints' begs the question how much additional 'artificial intelligence' is needed? Consequently, we will discuss chemometric strategies relevant to IR diagnostics along with selected application examples highlighting the transformation from analytical chemistry into digital analytical sciences.

A screening Test for Alzheimer's Disease Based on Raman Hyperspectroscopy and Machine Learning

Igor. K. Lednev - University at Albany, State University of New York, Albany, USA

Raman hyperspectroscopy combined with advanced statistics is uniquely suitable for characterizing microheterogeneous systems. Understanding the structure and (bio)chemical composition of samples at the microscopic level is important for many practical applications including material science, pharmaceutical industry, etc. We have recently demonstrated a great potential of Raman hyperspectroscopy for disease diagnostics. In this presentation, we will discuss the development of a novel, noninvasive approach for Alzheimer's disease (AD) diagnostics based on Raman spectroscopy of blood, cerebrospinal fluid and saliva. Near infrared (NIR) Raman hyperspectroscopy coupled with machine learning was utilized for differentiating patients diagnosed with Alzheimer's disease, other types of dementia and healthy control subjects with more than 95% sensitivity and specificity. When fully developed, this fast, inexpensive and noninvasive method could be used for screening at risk patient populations for AD development and progression.f Finland Ltd, Espo, Finland

Applications of AI-assisted vibrational spectroscopy: the development of the RamanBioAssay into a platform technology for cell interaction studies

Anja Silge, Leibniz Institute of Photonic Technology, Jena, Germany

APPLICATIONS OF AI-ASSISTED VIBRATIONAL SPECTROSCOPY – AGRICULTURE, FOOD, ENVIRONMENTAL MONITORING

6 March // 17 - 17:30 p.m. // S. Czapski

Chair: Boris Mizaikoff

NIR Spectroscopy in Phytopharmaceutical and Natural Drug Analysis – Robust Applications and Technological Advancements

Christian Huck - Leopold-Franzens University, Innsbruck, Austria

In the field of phytopharmaceuticals and natural drug analysis, Near-Infrared (NIR) spectroscopy serves as an indispensable tool for comprehensive sample evaluation on- and off-site. This technique, known for its non-destructive and rapid analysis capabilities, enables the examination of the molecular composition of herbal materials, extracts, and formulations and finds utility in ensuring the quality, efficacy, and safety of phytopharmaceuticals and natural drugs in phytopharmaceutical industry. Recent developments, including the application of portable, handheld spectrometers in the field, enhance the decision-making processes in the development, production, and quality assurance of phytopharmaceuticals and natural drugs [1].

The demand for plant-based medicines and natural remedies grows, with the global market of 87 billion USD (2022) and annual growth of 7%. The integration of NIR spectroscopy with phytopharmaceutical analysis becomes increasingly critical for its wide spectrum of capabilities offered in this sector including raw material identification, quantitative analysis of active compounds, product authentication, and in-field off-site applications such as plant growth monitoring and harvest time optimization.

This presentation explores the technical aspects of NIR spectroscopy in phytopharmaceutical analysis, including recent advances in the instruments, data-analysis, and specific applications. Emphasis is placed on studies assessing the analytical performance of miniaturized NIR spectrometers across various technologies. Furthermore, the integration of machine

learning and chemometric approaches with NIR spectroscopy for improved data analysis and predictive modeling is overviewed. This includes the application of Artificial Neural Networks (ANN) and non-linear regression methods, as well as the optimization of the entire analytical framework.

Reference:

1. Be ć, K.B.; Grabska, J.; Huck, C.W. J. Pharm. Biomed. Anal. 2021, 193, 113686

Handheld NIR Spectroscopy : A Rapid On-Site Technique for Quality Control and Protection against Counterfeiting in the Materials and Life Sciences

Heinz Siesler - University Duisburg-Essen, Essen, Germany

The presentation considers the rapid development of miniaturized handheld NIR spectrometers over the last decade and provides an overview of current instrumental developments and exemplary applications in the fields of materials and life sciences control as well as environmentally relevant investigations. Care is taken, however, not to fall into the over-optimistic narrative of some direct-to-consumer companies, which has raised unrealistic expectations with full-bodied promises, but has harmed the very valuable technology of NIR spectroscopy, rather than promoting its further development. Particular attention is paid to potential applications that will enable a clientele that is not necessarily scientifically trained to solve quality control and authentication problems in everyday life with this technology in the not-too-distant future.

Non-invasive, non-destructive and confirmatory diagnostics of pathogens in plants and seeds

Dmitry Kurouski - Texas A&M University, USA

Digital farming is a novel agricultural philosophy that aims to maximize a crop yield with the minimal environmental impact. Digital farming requires development of sensors that can work directly in the field providing information about the plant's health.

In this talk, I will show how Raman spectroscopy, an emerging analytical technique, can be used for non- invasive, non-destructive, and confirmatory diagnostics of diseases, as well as abiotic stresses in plants. I will also discuss the accuracy of Raman in plant phenotyping and assessment of nutritional content of grain. The talk will also demonstrate how Raman can be used for identification and digital selection of plants. These findings suggest that Raman can transform the agriculture in the U.S. allowing for automated, remote and chemical-free sensing of plant health directly in the field. phenotyping and assessment of nutritional content of grain. The talk will also demonstrate how Raman can be used for identification and digital selection of plants. These findings suggest that Raman can transform the agriculture in the U.S. allowing for automated, remote and chemical-free sensing of plant health directly in the field.

POSTER PRESENTATIONS

The poster exhibition is centrally located and can be visited all day from March 4 - 6. There will also be two sessions dedicated to viewing the posters. On March 5 and 6, all poster authors are asked to be available at their posters after lunch from 1:30 - 2 p.m. to answer questions.

ICOB-P-01 **General data pipeline for MALDI – TOF/ IMS and statistical analysis**
Mou Adhikari – Friedrich Schiller University Jena, Jena, Germany

ICOB-P-02 **Investigation of data fusion pipelines for correlation of photonic and clinical data**
Sultana Farhana Azam – Friedrich Schiller University Jena, Jena, Germany

ICOB-P-03 **Graphene Photonic Heterostructure Device for Biosensing**
Emir Aznakayev – National Aviation University, Kyiv, Ukraine

ICOB-P-04 **Nonlinear multimodal imaging towards endoscopic applications**
Hyeonsoo Bae – Leibniz Institute of Photonic Technology, Jena, Germany

ICOB-P-05 **Intraoperative Tumor Diagnosis in Head and Neck Cancer with Raman Spectroscopy: The Prospective Clinical Trial RAMAN-HNSCC**
Ayman Bali – University Hospital, Jena, Germany

ICOB-P-06 **Label-free Surface Enhanced Raman Scattering (SERS) of Different Proteins**
Shrobona Banerjee – Humboldt University Berlin, Berlin, Germany

ICOB-P-07 **Investigating microbiome-host interactions by combining marker-independent imaging with machine learning approaches in an Organ-on-a-Chip application**
Emanuel Behling – Eberhard Karls University Tübingen, Tübingen, Germany

ICOB-P-08 **Surface-enhanced Raman scattering of ergothioneine in biological samples.**
Alois Bonifacio – University of Trieste, Trieste, Italy

ICOB-P-09 **Fusion of food profiling data from various analytical techniques**
Kim Brettschneider – University Hamburg, Hamburg, Germany

ICOB-P-10 **Label-free Cancer Cell Death Monitoring by Stimulated Raman Microscopy**
Tim Hellwig – Refined Laser Systems GmbH, Münster, Germany

ICOB-P-11 **Rigid endomicroscopic system for cancer diagnosis and tissue removal**
Matteo Calvarese – Leibniz Institute of Photonic Technology, Jena, Germany

ICOB-P-12 **Fluorescence dynamics of Tb-DPA complexes**
Cristina Consani – Silicon Austria Labs GmbH, Villach, Austria

ICOB-P-13 **Uncertainty Quantification in AI using Monte Carlo Dropout for Raman Spectra Classification**
Jhonatan Contreras – Friedrich Schiller University Jena, Jena, Germany

ICOB-P-14 **Image evaluation method to optimize uneven illumination corrections in multimodal microscopy**
Elena Corbetta – Friedrich Schiller University Jena, Jena, Germany

ICOB-P-15 **Confocal Raman spectroscopic analysis of pathogen biofilms**
Dongyu Cui – Friedrich Schiller University Jena, Jena, Germany

ICOB-P-16 **Comprehensive Evaluation of Color Transformation Methods for H&E and Multimodal Images: A Focus on Stability**
Fatemeh Zahra Darzi – Friedrich Schiller University Jena, Jena, Germany

ICOB-P-17 **A systematic investigation of image pre-processing on image classification**
Pegah Dehbozorgi – Friedrich Schiller University Jena, Jena, Germany

ICOB-P-18 **Raman-based Detection of Natural Products in Microbial Communication**
Tony Dib – Leibniz Institute of Photonic Technology, Jena, Germany

ICOB-P-19 **Temporal analysis of Alkyne tagged DNA using surface enhanced Raman spectroscopy on silver dendritic structures**
Aradhana Dwivedi – Leibniz Institute of Photonic Technology, Jena, Germany

ICOB-P-20 **In silico analytics in vibrational spectroscopy**
Tarek Eissa – Ludwig Maximilians University Munich, Garching, Germany

ICOB-P-21 **Drug distribution and metabolism via label-free molecular fingerprint**
Samir Elmashtoly – Leibniz Institute of Photonic Technology, Jena, Germany

ICOB-P-22 **Cloud-Based System for Digital Pathology Image Analysis**
Rodrigo Escobar Diaz Guerrero – Leibniz Institute of Photonic Technology, Jena, Germany

ICOB-P-23 **Raman microspectroscopy for detecting head and neck tumour markers in body liquids**
Edoardo Farnesi – Friedrich Schiller University Jena, JENA, Germany

ICOB-P-24 **Exploring analytical parameters in profiling of liquid human biofluids with infrared molecular fingerprinting**
Frank Fleischmann – Ludwig Maximilians University Munich, Garching, Germany

ICOB-P-25 **Isolation of Bacteria from Wastewater and Identification by Raman Spectroscopy**
Sandra Baaba Frempong – Friedrich Schiller University Jena, Jena, Germany

ICOB-P-26 **Raman spectroscopic platform for the characterization of bacterial blood stream infections**
Richard Grohs – Leibniz Institute of Photonic Technology, Jena, Germany

ICOB-P-27 **Advancing Cardiac Diagnostics: Exploring Non-Invasive Optical Modalities for Myocardial Tissue Characterization**
Alexander Gümbel – University of Applied Sciences Jena, Jena, Germany

ICOB-P-28 **Systematic investigation on device drift for Raman spectroscopy and quality control**
Shuxia Guo – Leibniz Institute of Photonic Technology, Jena, Germany

ICOB-P-29 **Characterization of Toll-like Receptor Activation of Monocytes using Raman Microscopy**
Leah Haase – Leibniz Institute of Photonic Technology, Jena, Germany

ICOB-P-30 **Detection of protein modification in biological tissue caused by physical plasma as a tool to optimize label-free spectroscopic visualization of plasma effects in vivo**
Sybille Hasse – Leibniz Institute for Plasma Science and Technology, Greifswald, Germany

ICOB-P-31 **Development of a filter-based spectral imaging system for position- and wavelength-dependent detection of localized surface plasmons**
Andrē Heewig – Leibniz Institute of Photonic Technology, Jena, Germany

ICOB-P-32 **High-throughput multimodal imaging and spectroscopy system for the analysis of cells**
S M Miftahul Islam – Leibniz Institute of Photonic Technology, Jena, Germany

ICOB-P-33 **Identification of Pathogenic Microbials by Digital Live-Cell Reporter Assays**
Duyguhan Kozal – Leibniz Institute of Photonic Technology, Jena, Germany

ICOB-P-34 **Integrating Hyperspectral Imaging with Mixed Reality for Enhanced Medical Diagnostics and Treatment Planning**
Christian Krueger – University of Applied Sciences Jena, Jena, Germany

ICOB-P-35 **SERS-based detection of antibiotics and metabolites in pharmaceutical formulations and clinical-relevant matrices**
Chen Liu – Leibniz Institute of Photonic Technology, Jena, Germany

ICOB-P-36 **Deep Learning based 3D Raman Spectral Data Analysis for Colorectal Tissue Diagnosis**
Ruihao Luo – Friedrich Schiller University Jena, Jena, Germany

ICOB-P-37 **Application Perspectives of Spectroscopic Imaging with Broadband CARS**
Carl Messerschmidt – Leibniz Institute of Photonic Technology, Jena, Germany

ICOB-P-38 **Spectroscopic Analysis through Spider Plots: Harnessing Pre-trained Networks for Raman Classification**
Azadeh Mokari – Leibniz Institute of Photonic Technology, Jena, Germany

ICOB-P-39 **Siamese neural networks used in bacteria classification analysed by Raman Spectroscopy**
Sara Mostafapour – Friedrich Schiller University Jena, Jena, Germany

ICOB-P-40 **Broadband CARS hyperspectral imaging of cells and tissues using a deep-learning NRB removal approach**
Ryan Muddiman – Maynooth University, Maynooth, Ireland

ICOB-P-41 **DNA Microarray-based method of target gene analysis in Vancomycin resistant Enterococci**
Ibukun Elizabeth Osadare – Leibniz Institute of Photonic Technology, Jena, Germany

ICOB-P-42 **Droplet microfluidics autosampler for multimodal imaging microscopy**
Fabian Ott – Leibniz Institute of Photonic Technology, Jena, Germany

ICOB-P-43 **Label-free differentiation of antimicrobial resistance groups using Raman spectroscopy**
Aikaterini Pistiki – Friedrich Schiller University Jena, Jena, Germany

ICOB-P-44 **Stability of the fluorescence of DNA-stabilized silver clusters**
Uwe Pliquett – Institute for Bioprocess and Analytical Measurement Technology, Heilbad Heiligenstadt, Germany

ICOB-P-45 **Digital droplet-based microfluidic reporter assays for live cell analysis**
Cornelia Reuter – Leibniz Institute of Photonic Technology, Jena, Germany

ICOB-P-46 **Quantum efficiency analysis of Raman signal enhancement by a cratered gold colloid**
Iuliia Riabenko – V.N. Kharkiv Karazin National University, Charkiw, Ukraine

ICOB-P-47 **Biomedical Applications of Metabolic Two-Photon Excited Fluorescence Lifetime Microscopy**
Marko Rodewald – Leibniz Institute of Photonic Technology, Jena, Germany

ICOB-P-48 **Raman spectroscopic analysis of aerobic Bacillus and anaerobic Clostridium species**
Markus Salbreiter – Friedrich Schiller University Jena, Jena, Germany

ICOB-P-49 **A Deep Learning approach for detecting single division events of bacteria in microfluidic droplets imaged by angle-resolved scattered light imaging**
Arjun Sarkar – Leibniz Institute for Natural Product Research, and Infection Biology – Hans-Knöll-Institute, Jena, Germany

ICOB-P-50 **Exploring the wavenumber silent region for biological issues**
Constanze Schultz – Leibniz Institute of Photonic Technology, Jena, Germany

ICOB-P-51 Liquid crystal tunable filter and imaging-based localized surface plasmon resonance spectrometry utilizing DNA-based recognition elements
Florian Seier – Leibniz Institute of Photonic Technology, Jena, Germany

ICOB-P-52 **Development and Application of a High-Throughput Raman Spectroscopy System for Rapid Detection and Characterization of Microplastics**
Shiwani Shiwani – Leibniz Institute of Photonic Technology, Jena, Germany

ICOB-P-53 **Evaluation of 3D light sheet microscopy for visualization of corneal morphological changes and qualitative assessment of the entire eye.**
Axel Stoecker – HAWK University of Applied Science and Arts Goettingen, Goettingen, Germany

ICOB-P-54 **Characterization of the interaction of SARS-CoV-2 viruses and ACE2 receptor using surface plasmon resonance**
Astrid Tannert – Leibniz Institute of Photonic Technology, Jena, Germany

ICOB-P-55 **Parameters Influencing Metabolic Imaging of White Blood Cells**
Astrid Tannert – Leibniz Institute of Photonic Technology, Jena, Germany

ICOB-P-56 **Multimodal Optical Imaging in Ear Diagnostics**
Sven Urban – University of Applied Sciences Jena, Jena, Germany

ICOB-P-57 **Colorectal Cancer Discrimination Through Probes-based Raman Spectroscopy and Optical Coherence Tomography**
David Vasquez – Leibniz Institute of Photonic Technology, Jena, Germany

ICOB-P-58 **Molecule transfer into mammalian cells by single sub-nanosecond laser pulses**
Rainer Wittig – Institute for Laser Technologies in Medicine & Metrology at Ulm University, Ulm, Germany

ICOB-P-59 **Disease biomarker identification based on mid-infrared spectroscopy and machine learning**
Leiying Xie – Leibniz Institute of Photonic Technology, Jena, Germany

ICOB-P-60 **Spatial tissue protein MS modification mapping to facilitate spectroscopic approaches**
Kristian Wende – Leibniz Institute for Plasma Science and Technology, Greifswald, Germany

ICOB-P-61 **Label-free, chemically specific imaging with the Leica STELLARIS 8 CRS – a true multi-modal optical discovery instrument**
Volker Schweikhard – Leica Microsystems CMS GmbH, Mannheim, Germany

ICOB-P-62 **Advancements in FLIM: Comparative Analysis and New Methods for High-Resolution, Rapid Microenvironmental Imaging**
Thomas Kellerer – Munich University of Applied Sciences, Munich, Germany

ICOB-P-63 **Advancements in miRNA Detection: Harnessing the Potential of a Silicon Nitride Photonic Biosensing Platform**
Florenta Costache, Fraunhofer Institute for Photonic Microsystems IPMS, Dresden/DE

ICOPVS-P-01 **Development of a fast Push-Broom Imaging Raman Micro-Spectrometer for biological tissue**
Fernando J. Aguila Castro – Leibniz Institute of Photonic Technology, Jena, Germany

ICOPVS-P-02 **High resolution in hyperspectral data analysis from nanoscale IR spectroscopic imaging – a challenge!**
Maryam Ali – Friedrich Schiller University Jena, Jena, Germany

ICOPVS-P-03 **Photo-thermal Expansion of Nanostructured Surfaces in nano-IR spectroscopic imaging using Photo-induced Force Microscopy (PiF-IR)**
Shohely Tasnim Anindo – Institute of Condensed Matter Theory and Solid State Optics, Jena, Germany

ICOPVS-P-04 **Infrared spectral biomarkers of hypoxia in 2D and 3D cultures of endothelial cells.**
Anna Antolak – Jagiellonian University, Krakow, Poland

ICOPVS-P-05 **DFT study, Vibrational frequency, and biological analysis on Methyl 2-hydroxy-4-methoxy benzoate**
Shinthiya Mystica B – Madras Christian College, Chennai, India

ICOPVS-P-06 **About 10x faster image acquisition and two orders of magnitude faster tuning in SRS microscopy including the fingerprint region of relevant biological samples**
Matthias Baudisch – APE Angewandte Physik and Elektronik GmbH, Berlin, Germany

ICOPVS-P-07 **Clinical-compatible stimulated Raman imaging device for intraoperative histology of fresh tissue samples**
Tim Hellwig – Refined Laser Systems GmbH, Münster, Germany

ICOPVS-P-08 **Tailoring the Cavity-Induced Interplay of Modes to Enhance Four-Wave Mixing over a Broadband Molecular Fingerprint Regime**
Abhik Chakraborty – Friedrich Schiller University Jena /
Leibniz Institute of Photonic Technology, Jena, Germany

ICOPVS-P-09 **Precision-Engineered Nanostar Arrays for Enhanced SERS Analysis**
Alexandre Chicharo – Humboldt University Berlin, Berlin, Germany

ICOPVS-P-10 **Deciphering the effect of solvent polarity and wavepacket dynamics in TADF emitting molecule using Transient absorption and ultrafast Raman Loss spectroscopy**
Nishant Dhiman – Indian Institute of Science Bangalore, Bangalore, India

ICOPVS-P-11 **Spectroscopic imaging of Fabry disease-associated lipid accumulations in cardiac cells**
Johann Dierks – Leibniz Institute for Analytical Sciences - ISAS e.V., Dortmund, Germany

ICOPVS-P-12 **Quantitative and computational analysis, molecular docking studies, and in-vitro assays on 4-Isopropylbenzoic acid: A potential anti-parkinsonian drug**
Eunice E – Madras Christian College, Chennai, India

ICOPVS-P-13 **Data-driven infrared molecular fingerprinting: From in silico modeling to establishing a population-wide health screening platform**
Tarek Eissa – Ludwig Maximilians University Munich, Garching bei München, Germany

ICOPVS-P-14 **Application of surrogate minimal depth to unravel surface-enhanced Raman scattering data**
Florian Gärber – University of Hamburg, Hamburg, Germany

ICOPVS-P-15 **Pregnancy Detection Based on Serum Samples Raman Spectroscopy**
Jose Luis Gonzales Solis – Culagos, Guadalajara University, Lagos de Moreno, Mexico

ICOPVS-P-16 **Development of a system for multispectral characterization of chyme in newborns**
Konstantin Gramatte – University of Applied Sciences Jena, Jena, Germany

ICOPVS-P-17 **A mid-IR spectroscopic setup for identifying viruses in human saliva under high throughput conditions**
Jonas Grzesiak – German Aerospace Center (DLR), Hardthausen, Germany

ICOPVS-P-18 **Deep tissue single laser source multimodal microscopy**
Gregor Hehl – Helmut Schmidt University, Hamburg, Germany

ICOPVS-P-19 **Rapid electric-field molecular fingerprinting for infrared phenotype diagnostics**
Philip Jacob – Max Planck Institute of Quantum Optics, Garching, Germany

ICOPVS-P-20 **Portable confocal POCT Raman spectrometer for biological/biomedical applications**
Izabella Jahn – Leibniz Institute of Photonic Technology, Jena, Germany

ICOPVS-P-21 **Autofluorescence spectral analysis for detecting urinary stone composition in emulated intraoperative ambient**
Hongbo Jia – Leibniz Institute for Neurobiology, Magdeburg, Germany

ICOPVS-P-22 **Effect of non-resonant background on the CARS data analysis**
Rajendhar Junjuri – Leibniz Institute of Photonic Technology, Jena, Germany

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Shravan Raghunathan – Leibniz Institute of Photonic Technology, Jena, Germany

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Josē Javier Ruiz – ICFO – Institute of Photonic Sciences, Castelldefels, Barcelona, Spain

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Kaleeswaran S – Madras Christian College, Chennai, India

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Artem Shydliukh – Leibniz Institute of Photonic Technology, Jena, Germany

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Anooj Thayyil Raveendran – Leibniz Institute of Photonic Technology, Jena, Germany

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Liudmila Voronina – Ludwig Maximilians University Munich, Garching bei München, Germany

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Manja Marz – Friedrich Schiller University Jena, Jena, Germany

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