

# MINERVA-GENTNER SYMPOSIA 2023



## **"Bringing the Sea to Berlin"**

**The future of marine sciences building on high-resolution  
X-ray characterization methods at synchrotrons**

**19 to 21 June 2023**

**Lecture hall "KINO" at HZB building 13.10 (Magnusstraße 2)**

The Minerva-Gentner Symposium is a format to bring together Israeli scientists with colleagues from Germany and other countries through conferences, workshops etc. The format is named after the physicist and former director of the Max Planck Institute for Nuclear Physics, Wolfgang Gentner, who was a member of the first German scientific delegation to Israel in 1959 and later member of the board of the Weizmann-Institute in Rehovot.

Minerva-Gentner Symposia are intended to enable scientific discourse, exchange of ideas, and new interactions in a given field of research. Furthermore, the Symposia should initiate new collaborative efforts in fields that are that are highly innovative and not yet in the focus of German-Israeli cooperation.

A typical Minerva-Gentner Symposium has about 25-50 participants. The invited scientists should come from various institutions in Germany and Israel. In addition to the Israeli and German participants, also scientists from other countries can be included in the program. Not yet established but promising young scientists (PhD-students, Post-Docs) shall have the opportunity to get in contact with senior scientists during these symposia. (<https://www.minerva.mpg.de/19287/gentner-symposia>)

## PROGRAMME DAY 1 / 19 June 2023 / Monday

13:00 - 14:00	Registration	KINO Foyer
14:00 - 14:30	OPENING REMARKS - Tali Mass, Antje Vollmer & Paul Zaslansky	KINO
<b>14:30 - 15:30</b>	<b>SESSION I: Marine science meets Synchrotron science / Overview</b>	<b>KINO</b>
14:30 - 15:00	<b>Peter Fratzl</b> Synchrotron studies of multiscale biomaterial behaviour	
15:00 - 15:30	<b>Gert Weber</b> Global plastic pollution and routes towards a sustainable circular economy for synthetic polymers	
<b>15:30 - 17:10</b>	<b>SESSION II: Marine questions / Part I</b>	<b>KINO</b>
15:30 - 15:50	<b>Jaroslav Stolarski</b> The so-called pristine preservation of fossil carbonate biominerals: myths and facts	
15:50 - 16:10	<b>Igor Zlotnikov</b> Dynamics of Topological Defects and Structural Synchronization in Forming Nacre	
16:10 - 16:30	<b>Tobias Primel</b> Multiscale correlative imaging of mussel byssus fabrication	
16:30 - 16:50	<b>Stuart Stock</b> Micro- and nanostructure of the mineralized centra of shark vertebrae	
16:50 - 17:10	<b>Hadar Shaked</b> Inhomogeneous Mg distribution within high Mg bearing mineralized tissues	
17:10 - 17:30	Coffee Break	KINO Foyer
<b>17:30 - 18:30</b>	<b>SESSION III: Synchrotron landscape</b>	<b>KINO</b>
17:30 - 18:00	<b>Antje Vollmer</b> The synchrotron radiation source BESSY II - research options for the international science community	
18:00 - 18:30	<b>Andrea Lausi</b> SESAME - Light for the middle east	
<b>18:30 - 20:00</b>	<b>Guided Tours / BESSY II Experimental Hall</b>	
<b>20:00 - 22:30</b>	<b>POSTER SESSION / Part I</b>	<b>KINO Foyer</b>

### SESSION I: Marine science meets synchrotron science / Overview

#### Synchrotron studies of multiscale biomaterial behavior

Peter Fratzl ([Peter.Fratzl@mpikg.mpg.de](mailto:Peter.Fratzl@mpikg.mpg.de))

*Max Planck Institute of Colloids and Interfaces, Department of Biomaterials, Potsdam Science Park, Am Mühlenberg 1, 14424 Potsdam OT Golm, Germany*

Biological materials acquire many of their remarkable properties through hierarchical structuring. Synchrotron radiation provides a number of tools for in-operando analysis of multiscale structure as a function of external parameters, such as mechanical load, humidity or temperature. Many scales from molecular dimensions to the millimeter scale can be characterized through scanning diffraction, scattering and imaging in 2D as well as through tomographic methods in 3D. Several examples of marine and terrestrial biological materials will be discussed.

## **Global plastic pollution and routes towards a sustainable circular economy for synthetic polymers**

Gert Weber ([gert.weber@helmholtz-berlin.de](mailto:gert.weber@helmholtz-berlin.de))

*Helmholtz-Zentrum Berlin, Albert-Einstein-Str. 15, 12489 Berlin, Germany*

Despite many advantages during their lifetime, disposed synthetic polymers (plastics) have turned into a global environmental burden for terrestrial and marine environments. Plastics deteriorate to micro- or nanometer-sized particles, found even in remote regions, like the deep sea or the North Pole. This is an alarming development and solutions are urgently needed, starting with appreciating disposed plastics as valuable goods. Due to similarities of natural and synthetic polymers, enzymes appear a sustainable alternative to current recycling processes fostering a circular plastic economy.

## **SESSION II: Marine questions / Part I**

### **The so-called pristine preservation of fossil carbonate biominerals: myths and facts**

Jaroslawn Stolarski ([stolacy@twarda.pan.pl](mailto:stolacy@twarda.pan.pl))

*Institute of Paleobiology, Polish Academy of Sciences, Twarda 51/55, 00-818 Warsaw, Poland*

This is not a formal abstract yet: using modern and fossil coral/fish otolith examples of calcium carbonate biominerals I would to address the problem of common paleontological myth on "pristine" preservation of fossils.

### **Dynamics of Topological Defects and Structural Synchronization in Forming Nacre**

Igor Zlotnikov ([igor.zlotnikov@tu-dresden.de](mailto:igor.zlotnikov@tu-dresden.de))

*B CUBE - Center for Molecular Bioengineering, Technische Universität Dresden, Germany*

Molluscan shells ultrastructures are a paradigm of complex hierarchical biocomposite structures formed in the course of extracellular biomineralization. Morphogenesis of these ultrastructures is known to follow thermodynamically driven self-assembly processes in accordance with the principles of classical materials science. Sheet nacre ultrastructure is a highly regular and periodic architecture composed of thin organic membranes and aragonitic layers, which are made of flat mesocrystalline platelets. Similar to classical crystal growth, nacre deposition is accompanied by incorporation of two-dimensional defects, such as dislocations and twinning, that are integral to its formation process. However, in contrast to a generic atomic-scale lattice, in sheet nacre, these defects occur on the mesoscale level. Specifically, twinning in aragonite is known to be responsible for the shape of nacre platelets and structural dislocations in the layered assembly are key to its morphogenesis. In the present work, we employ synchrotron-based nanotomographic imaging combined with machine learning post-processing techniques to visualize and understand the nature and the dynamics of mesoscale dislocations in the nacre of the bivalve *Unio pictorum* in 3D. By drawing an analogy to processes in classical materials science, we shed light on the role of structural dislocations and their interaction in sheet nacre formation. This work is a step towards a deeper understanding of fundamental thermodynamic and kinetic principles that drive the self-assembly of nacre.

## **Multiscale correlative imaging of mussel byssus fabrication**

Tobias Priemel ([tobias.priemel@mail.mcgill.ca](mailto:tobias.priemel@mail.mcgill.ca))

*McGill University, Sherbrooke Street West 801, H3A 0B8 Montreal, Canada*

To adhere to rocky seashore habitats, marine mussels use a specialized organ known as the foot to produce strong, underwater adhesive fibers called a byssal threads. During the fabrication process, which is similar to injection molding, more than 15 different proteins are secreted into the mussel foot groove where they assemble into a hierarchically organized fiber. By using a combination of various imaging techniques including microCT, electron and Raman microscopy as well as X-ray fluorescence, we gained critical insights into the machinery used in the fabrication process and the dynamics of secretion

## **Micro- and nanostructure of the mineralized centra of shark vertebrae**

Stuart Stock ([s-stock@northwestern.edu](mailto:s-stock@northwestern.edu))

*Feinberg School of Medicine, Northwestern University, 302 E. Huron St., Simpson Querrey Bldg., 8th Floor, 60611 Chicago, USA*

Shark vertebrae survive in vivo strains greater than 4% for millions of loading cycles without a repair mechanism like that of remodeling in bone. This talk presents results from synchrotron microCT, x-ray diffraction and small angle scattering mapping in 2D and 3D and x-ray fluorescence mapping. We find that the microstructure of the mineralized cartilage consists of interconnected trabeculae. Further, the bioapatite mineral phase differs somewhat from bone and dentin and has strong crystallographic texture.

## **Inhomogeneous Mg distribution within high Mg bearing mineralized tissues**

Hadar Shaked ([shadar3@gmail.com](mailto:shadar3@gmail.com))

*The faculty of materials science and engineering - Technion, Technion 1, 3200003 Haifa, Israel*

Biomineralization is the process by which organisms form minerals in nature. There are many pathways by which organisms form biominerals; saturated solutions, organic matrix-mediated mineralization, matrix vesicle mineralization, amorphous-to-crystalline transformation, etc. The use of an amorphous precursor is especially common in the deposition of calcium carbonate's (CaCO<sub>3</sub>) metastable phase – amorphous calcium carbonate (ACC). An additive frequently seen in CaCO<sub>3</sub> biominerals is Mg, which can be incorporated in rates as high as 40 at.%, much higher than its thermodynamic stability of ~2at.%. Previous studies have shown that biomineralized tissues can be divided into two groups based on their Mg content; biominerals containing Mg concentrations higher than 14 mol% probably go through a spinodal decomposition in the formation stage, while those with lower concentrations do not. The spinodal decomposition leads to the formation of Mg-rich inclusions within a Mg-poor matrix. In TEM the Mg-rich areas can be seen as higher contrast areas in the matrix, yet due to their nanometric size and low relative contrast, little was known about their chemical composition and their integration within the matrix. By using synchrotron radiation both at the ESRF (ID 16A) and at BESSY | (U41-TXM) herein we will present a detailed analysis of the elements within high Mg-bearing organisms, focusing mainly on the brittle star *Ophiomastix wendtii* (*O. wendtii*). For the first time, we identified the exact chemical composition of the coherent Mg-rich inclusions within the *O. wendtii* low-Mg calcite matrix as magnesite.

## **SESSION III: Synchrotron landscape**

### **The synchrotron radiation source BESSY II - research options for the international science community**

Antje Vollmer ([antje.vollmer@helmholtz-berlin.de](mailto:antje.vollmer@helmholtz-berlin.de))

*Helmholtz-Zentrum Berlin, Albert-Einstein-Str. 15, 12489 Berlin, Germany*

BESSY II, the synchrotron radiation facility in Berlin, Germany, offers a broad variety of research options for the international scientific community free of charge. From photovoltaics, chemical energy conversion, batteries to quantum materials, information technology materials, biology, cultural heritage and medical research we provide infrastructure for your scientific projects. Although BESSY II is dedicated to soft X-ray regime, experiments using infrared radiation on the low energy side and tender or even hard X-rays on the other are feasible. The instrument portfolio allows a multitude of methods like photoemission, photoabsorption, scattering and diffraction methods, microscopies or imaging. BESSY II is a key enabler for developing solutions to the grand global challenge societies are facing, namely the progressing climate crisis, and the urgent need for sustainable, carbon-neutral energy. However, global problems have to be addressed globally; with international knowledge exchange, “brain-circulation”, and cooperation we can contribute to tackling global problems.

### **SESAME - LIGHT FOR THE MIDDLE EAST**

Andrea Lausi ([Andrea.lausi@sesame.org.jo](mailto:Andrea.lausi@sesame.org.jo))

*SESAME, Mohamad Majed Aletan Street 7, 11822 Amman, Jordan*

Officially opened in Jordan in May 2017, SESAME (Synchrotron-light for Experimental Science and Applications in the Middle East) is a cooperative venture by scientists and governments of the region, and the region's first major international centre of excellence for research. The need for an international light source in the Middle East was first recognised by the Pakistani Nobel Laureate Abdus Salam and by the Middle East Scientific Cooperation (MESOC) group. Nowadays, SESAME is a third-generation synchrotron light source with three beamlines already open to users, and two under commissioning.

## PROGRAMME DAY 2 / 20 June 2023 / Tuesday

<b>09:00 - 10:40</b>	<b>SESSION IV: Synchrotron Methods / Part I</b>	<b>KINO</b>
09:00 - 09:20	<b>Ivo Zizak</b> Multimodal X-ray methods at mySpot	
09:20 - 09:40	<b>Karpov Dmitry</b> Nanoscale X-ray fluorescence and phase contrast bio-imaging at ID16A of the ESRF-EBS	
09:40 - 10:00	<b>Emanuel Schneck</b> Element-specific structural characterization of bimolecular layers and interfaces with standing-wave x-ray fluorescence	
10:00 - 10:20	<b>Alexander Rack</b> Microtomography Beamline ID19	
10:20 - 10:40	<b>Stefan Werner</b> Transmission X-ray Microscopy for nanoscale soft and tender Spectromicroscopy and Tomography	
10:40 - 11:10	Coffee Break	KINO Foyer
<b>11:10 - 12:10</b>	<b>SESSION V: Marine questions / Part II</b>	<b>KINO</b>
11:10 - 11:30	<b>Ariel Chazan</b> Functional metagenomics and microbial rhodopsins	
11:30 - 11:50	<b>Giuseppe Falini</b> Effects of intra-skeletal organic matrix in coral calcification process	
11:50 - 12:10	<b>Marthe Rousseau</b> Nacre (not only a beautiful material but also a biomaterial) under the X-rays	
12:10 - 16:00	Lunch Break & Networking Time	Canteens on-site
16:00 - 16:30	Coffee Break	KINO Foyer
<b>16:30 - 17:50</b>	<b>SESSION VI: Synchrotron methods / Part II</b>	<b>KINO</b>
16:30 - 16:50	<b>Gianluca Lori</b> BEATS: synchrotron computed tomography for the Middle East	
16:50 - 17:10	<b>Manfred Weiss</b> Fragment-Screening at the Helmholtz-Zentrum Berlin	
17:10 - 17:30	<b>Lili Puskar</b> Infrared beamline IRIS for the applications on Marine science	
17:30 - 17:50	<b>Ioanna Mantouvalou</b> Combined laboratory and synchrotron studies for elemental imaging from the nano- to the millimeter scale	
17:50 - 18:20	Coffee Break	KINO Foyer
<b>18:20 - 20:00</b>	<b>SESSION VII: Marine questions / Part III</b>	<b>KINO</b>
18:20 - 18:40	<b>Dvir Gur</b> The Cellular Regulation of Molecular Crystal-Forming Cells	
18:40 - 19:00	<b>Oliver Späker</b> XRD/XRF mapping reveals cuticle modifications of <i>Limulus polyphemus</i> cornea leading to RI gradients	
19:00 - 19:20	<b>Noy Shaked</b> Studying guanine biomineral function in the green alga <i>Phacotus lenticularis</i>	
19:20 - 19:40	<b>Amir Sagi</b> Broad view of molt cycle, related gene expression and biomineralization in crayfish	
19:40 - 20:00	<b>Avital Wagner</b> Functional Molecular Crystals in Marine Biology	
<b>20:00 - 22:30</b>	<b>POSTER SESSION / Part II</b>	<b>KINO Foyer</b>

## SESSION IV: Synchrotron Methods / Part I

### Multimodal X-ray methods at mySpot

Ivo Zizak ([zizak@helmholtz-berlin.de](mailto:zizak@helmholtz-berlin.de))

*Helmholtz-Zentrum-Berlin, Albert-Einstein-Str. 15, 12489 Berlin, Germany*

Presenting the mySpot, a versatile X-ray scanning station with micrometer resolution, as well as some examples of measured results. A combination of methods can be performed simultaneously at the same sample position. It is especially designed for (but not limited to) hierarchically structured biological samples. Structural information from different scales (XRD, SAXS, microscope) can be combined with chemical information (XRF, EXAFS, XANES) and molecular information (Raman) providing unique insight into the mutual dependencies of different parameters and their distribution across the sample.

### Nanoscale X-ray fluorescence and phase contrast bio-imaging at ID16A of the ESRF-EBS

Dmitry Karpov ([dmitry.karpov@esrf.fr](mailto:dmitry.karpov@esrf.fr))

*European Synchrotron Radiation Facility (ESRF), Avenue des Martyrs 71, 38000 Grenoble, France*

The ID16A beamline is at the forefront of the hard X-ray microscopy with its unique instrumentation successfully applied to studies of biomineralization, cellular biology, and in neural imaging to name a few. Recent ESRF-EBS upgrade allows us to further push the resolution to 3D sub-50 nm both for electron density and elemental composition. In this talk I will present our recent contributions to understanding of geometrical frustrations in sponges, self-assembly processes, and electron conductivity in cable bacteria. I will focus on what the beamline can offer to the marine sciences community.

### Element-specific structural characterization of biomolecular layers and interfaces with standing-wave x-ray fluorescence

Emanuel Schneck ([emanuel.schneck@pkm.tu-darmstadt.de](mailto:emanuel.schneck@pkm.tu-darmstadt.de))

*TU Darmstadt, Hochschulstrasse 8, 64289 Darmstadt, Germany*

In nature, biomolecules are often organized as functional thin layers in interfacial architectures, the most prominent examples being biological membranes. Biomolecular layers play also important roles in context with biotechnological surfaces, for instance when they are the result of adsorption processes. For the understanding of many biological or biotechnologically relevant processes, detailed structural insight into the involved biomolecular layers is required. Here, we use standing-wave x-ray fluorescence [1, 2] to localize chemical elements in solid-supported lipid and protein layers.



## **Microtomography Beamline ID19**

Alexander Rack ([rack@esrf.fr](mailto:rack@esrf.fr))

*European Synchrotron Radiation Facility (ESRF), Avenue des Martyrs 71, 38043 Grenoble, France*

Beamline ID19 of the ESRF operates experimental facilities located 150 m downstream of the source: the long distance suppresses the influence of the finite sources size on the image formation and hence, allows one to exploit propagation-based phase contrast. Frequently, polychromatic configurations are applied as the increased bandwidth leads to drastically reduced exposure times, while the absence of (reflection) X-ray optical elements increases the imaging sensitivity. Ideal conditions to image fine-detailed samples which high resolution and high contrast.

## **Transmission X-ray Microscopy for nanoscale soft and tender Spectromicroscopy and Tomography**

Stephan Werner ([stephan.werner@helmholtz-berlin.de](mailto:stephan.werner@helmholtz-berlin.de))

*Helmholtz-Zentrum Berlin, Albert-Einstein-Str. 15, 12489 Berlin, Germany*

The Helmholtz-Zentrum Berlin (HZB) operates a transmission X-ray microscope (TXM) for nanoscale soft and tender X-ray imaging at the U41-PGM1 undulator beamline at BESSY II. The advanced optical setup of the HZB-TXM permits spectromicroscopic applications as well as correlative fluorescence and nanoscale tomographic imaging of cryogenic samples. We will discuss the unique imaging capabilities of the HZB-TXM and give an overview of recent results in material, energy and life sciences. We will also report on new approaches to increase the 2D and 3D resolution for soft and tender X-ray microscopy.

## **SESSION V: Marine questions / Part II**

### **Functional metagenomics and microbial rhodopsins**

Ariel Chazan ([ariel.ch@campus.technion.ac.il](mailto:ariel.ch@campus.technion.ac.il))

*Technion, Technion 1, 3200003 Haifa, Israel*

Two metagenomic discoveries of light harvesting by microorganisms will be discussed in my lecture. The first is the finding of light-driven rhodopsin proton pumps in marine microorganisms. The second is the discovery of carotenoid antennas that can bind aquatic microbial rhodopsins from the outside and transfer energy captured in the blue light range to the retinal molecule within the rhodopsin. This can increase light capture in about 40%. The implications of microbial rhodopsins to oceanic and lake phototrophy will be discussed.

### **Effects of intra-skeletal organic matrix in coral calcification process**

Giuseppe Falini ([giuseppe.falini@unibo.it](mailto:giuseppe.falini@unibo.it))

*Alma Mater Studiorum - University of Bologna, Via Selmi 2, 40126 Bologna, Italia*

The presentation will report the summary of several researches on the effects of the whole intra-skeletal coral organic matrix (OM) from different species on the formation of calcium carbonate. Different experimental strategies of calcium carbonate synthesis will be presented. Particular attention will be paid on the influence of magnesium ions in the process of calcium carbonate formation. The obtained results will show that, although the compositional characteristics of the OM from different species are similar, their effect on the formation of calcium carbonate varies drastically.

## **Nacre (not only a beautiful material but also a biomaterial) under the X-rays**

Marthe Rousseau ([marthe.rousseau@univ-st-etienne.fr](mailto:marthe.rousseau@univ-st-etienne.fr))

*U1059 INSERM - SAINBIOSE, Rue de la Marandière 10, 42270 Saint-Priest-en-Jarez, France*

Nacre, also called mother-of-pearl, is one of the most beautiful marine substance, produced by mollusks. An overview will be presented about the contribution of synchrotron to the study of nacre structure and formation mechanism. It will be followed by the open challenges in this field and how high-resolution X-ray characterization methods at synchrotrons could help to answer. Furthermore nacre presents osteogenic properties. Recently absorption and phase contrast enhanced tomography on BAMline at BESSY was used to investigate sham and mother-of-pearl powder filling-in bone defects in sheep.

## **SESSION VI: Synchrotron methods / Part II**

### **BEATS: synchrotron computed tomography for the Middle East**

Gianluca Iori ([gianluca.iori@sesame.org.jo](mailto:gianluca.iori@sesame.org.jo))

*Synchrotron Light for Experimental Science and Applications in the Middle East (SESAME), Allan P.O. box 7, 19252 Allan, Jordan*

The BEAmline for Tomography at SESAME (BEATS) operates a full-field X-ray micro tomography station providing service to scientists from archaeology, cultural heritage, medicine, biology, geology, materials and environmental sciences. The beamline has a total length of 45 m, and an insertion device providing high photon flux and a usable beam size of 70×15 mm<sup>2</sup> at the sample. Filtered white and monochromatic beam modalities are available. In my contribution, I will present the design, installation, commissioning and inauguration of the first synchrotron microCT station in the Middle East.

### **Fragment-Screening at the Helmholtz-Zentrum Berlin**

Manfred Weiss ([msweiss@helmholtz-berlin.de](mailto:msweiss@helmholtz-berlin.de))

*Helmholtz-Zentrum Berlin, Albert-Einstein-Str. 15, 12489 Berlin, Germany*

Fragment screening is a technique that helps to identify promising starting points for ligand design. Given that suitable crystals of the protein of interest are available and exhibit reproducibly good X-ray diffraction properties, X-ray crystallography is nowadays probably the preferred method for fragment screening, because - in addition to a simple yes/no answer with respect to binding - it provides detailed 3D information of the binding mode.

### **Infrared beamline IRIS for the applications on Marine science**

Ljiljana Puskar ([ljiljana.puskar@helmholtz-berlin.de](mailto:ljiljana.puskar@helmholtz-berlin.de))

*Helmholtz-Zentrum Berlin, Albert-Einstein-Str. 15, 12489 Berlin, Germany*

Infrared spectroscopy at the IRIS beamline provides chemical information on the small areas of heterogeneous samples from a wide range of materials including thin films or layers, single biological cells or tissues. IRIS overview will be given with particular focus on the relevance to the marine science applications. Investigation of materials with diffraction-limited spatial resolution (~5 microns) is achieved by the FTIR-micro-spectroscopy station. When chemical information at the nanoscale (~20 nm) is desired our near-field microscopy station is utilized.

## **Combined laboratory and synchrotron studies for elemental imaging from the nano- to the millimeter scale**

Ioanna Mantouvalou ([ioanna.mantouvalou@helmholtz-berlin.de](mailto:ioanna.mantouvalou@helmholtz-berlin.de))

*Helmholtz-Zentrum Berlin, Albert-Einstein-Str. 15, 12489 Berlin, Germany*

Elemental imaging with X-ray excitation offers a wide range of possible applications. The non-destructive nature of X-rays and the possibility to image matter in three dimensions due to their high penetration depth can be exploited for successive or simultaneous investigations. In this presentation, we demonstrate the synergies offered by the combination of using synchrotron radiation instrumentation for specialized analysis and laboratory instrumentation for statistically relevant studies for the analysis of specimens from (marine) biology.

## **SESSION VII: Marine questions / Part III**

### **The Cellular Regulation of Molecular Crystal-Forming Cells**

Dvir Gur ([dvir.gur@weizmann.ac.il](mailto:dvir.gur@weizmann.ac.il))

*Weizmann Institute of Science, 234 Herzl Street, 706001 Rehovot, Israel*

Organisms use guanine crystals which are formed by specialized cells dubbed iridophores for an astonishing variety of functions. In iridophores crystallization takes place within a unique organelle where control of crystal size and shape far exceeds our abilities to grow crystals synthetically. The cellular mechanisms regulating this process remain unknown. Using proteomics together with state-of-the-art cryo-imaging, synchrotron-based WAXS and XANS, we were able to characterize the early stages of intracellular crystal formation in fish, and identify the key participating machinery.

### **XRD/XRF mapping reveals cuticle modifications of *Limulus polyphemus* cornea leading to RI gradients**

Oliver Späker ([oliver\\_christian.spaecker@tu-dresden.de](mailto:oliver_christian.spaecker@tu-dresden.de))

*B CUBE, TU Dresden, Tatzberg 41, 01307 Dresden, Germany*

The lateral compound eye of the horseshoe crab, *Limulus polyphemus*, contains cuticular cones focusing light on photoreceiving units. Correlating RI measurements of these specialized cuticle structures with high resolution XRD/XRF mapping allowed to identify structural and compositional variations leading to the observed RI. These are namely gradients in chitin/protein ratio, hydration and bromine doping. The study clarified the light focusing mechanism of this cuticle-based visual system, as well as identify modifications present in this versatile biomaterial in an optical context.

### **Studying guanine biomineral function in the green alga *Phacotus lenticularis***

Noy Shaked ([noy.shaked@weizmann.ac.il](mailto:noy.shaked@weizmann.ac.il))

*Weizmann Institute of Science, 234 Herzl Street, 7630031 Rehovot, Israel*

Guanine crystal assemblies fulfilling optical functions are widespread in multicellular organisms. In unicellular organisms, their function is unclear. Here, we documented guanine crystal distribution, orientation, and morphology in the algae *P. lenticularis* after phosphate depletion, using cryo-soft-Xray tomography and N-near-edge-spectroscopy. We produced 3D reconstructions of 40 whole cells and localized the guanine crystal inclusions. We observed high variability in cluster sizes, locations, crystal size, shape, and orientation, suggesting that guanine crystals most likely serve as nitrogen storage

### **Broad view of molt cycle, related gene expression and biomineralization in crayfish**

Amir Sagi ([sagia@bgu.ac.il](mailto:sagia@bgu.ac.il))

*Ben-Gurion University, PoB 653 BGU 1, 84105 Beer Sheva, Israel*

### **Functional Molecular Crystals in Marine Biology**

Avital Wagner ([avitalwa@post.bgu.ac.il](mailto:avitalwa@post.bgu.ac.il))

*Ben-Gurion University of the Negev, Ben-Gurion Blvd. 1, 8410501 Beer-Sheba, Israel*

Crystals of small organic molecules create many spectacular colors and visual phenomena in marine animals. Guanine crystals are ubiquitous in nature, and though their optics are well-understood, much remains unknown about how guanine crystals form. More recently, lesser known, isoxanthopterin crystals were found in decapod crustaceans. In this talk, we will discuss the connection between morphology, structure, and assembly of guanine and isoxanthopterin crystals in different biological systems, exploring both how guanine crystals form and how isoxanthopterin crystals are used to create structural colors

## PROGRAMME DAY 3 / 21 June 2023 / Wednesday

<b>09:00 - 10:20</b>	<b>SESSION VIII: Marine questions / Part IV</b>	<b>KINO</b>
09:00 - 09:20	<b>Shai Shaked</b> Two interesting instances of genes/proteins with respect to exoskeleton mineralization in crustaceans	
09:20 - 09:40	<b>Benjamin Kruppke</b> Crustacean proteins for modification of chitinous scaffolds – bioinspired bone substitute research	
09:40 - 10:00	<b>Tal Luzzatto</b> The new kid on the block: Exploring the migration route, physiology and metabolome of the invasive seaweed <i>Asparagopsis taxiformis</i>	
10:00 - 10:20	<b>Rodriguez Palomo Adrian</b> Structure of narwhal tusk studied by X-ray dark field imaging	
10:20 - 10:50	Coffee Break	KINO Foyer
<b>10:50 – 11:50</b>	<b>SESSION IX: Marine questions / Part V</b>	<b>KINO</b>
10:50 - 11:10	<b>Henrik Birkedal</b> Biomineralization of Mantis Shrimp Dactyl Club during Development	
11:10 - 11:30	<b>Ernesto Scoppola</b> Structure and Composition of biomaterials investigated by X-ray Scattering and Fluorescence Tomography	
11:30 - 11:50	<b>Marie Albéric</b> The concomitant role of amorphous calcium carbonate and organic molecules in forming colourful sea urchin single crystalline biominerals with convoluted porous structures	
<b>11:50 - 12:30</b>	<b>General Discussion &amp; Summary</b>	<b>KINO</b>

### SESSION VIII: Marine questions / Part IV

#### Two interesting instances of genes/proteins with respect to exoskeleton mineralization in crustaceans

Shai Avraham Shaked ([shaiavsh@post.bgu.ac.il](mailto:shaiavsh@post.bgu.ac.il))

*Ben-Gurion University of the Negev, Ben-Gurion Blvd 1, 8410501 Beer Sheva, Israel*

Phosphate transporter and structural proteins in the exoskeleton of a crayfish. Insights on molt cycle related expression patterns and mineralization.

#### Crustacean proteins for modification of chitinous scaffolds – bioinspired bone substitute research

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Chitin-based materials are well known for their biocompatibility and the processability to gels, films, porous scaffolds, fibers, etc. with classical methods (top-down or bottom-up) or additive manufacturing. This opens up an enormous potential for use as a degradable biomaterial. Our research focuses on the interaction of manufactured materials with tissue cells of bone remodeling. This is significantly influenced directly but also indirectly (via mineral formation) by proteins and peptides involved in the mineralization process of crustaceans, to be used for influencing tissue regeneration.

### **The new kid on the block: Exploring the migration route, physiology and metabolome of the invasive seaweed *Asparagopsis taxiformis***

Tal Luzzatto Knaan ([tluzzatto@univ.haifa.ac.il](mailto:tluzzatto@univ.haifa.ac.il))

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The red macroalgae *Asparagopsis taxiformis* (Delile) Trevisan (Bonnemaisoniales, Rhodophyta) is a highly invasive seaweed in temperate regions and is considered to be one of the 'worst invasive alien species threatening marine biodiversity in Europe'. With the seawater temperature rising, *A. taxiformis* is found to settle in new territories, repressing local fauna. In the Mediterranean Sea, two cryptic lineages were reported before the opening of the Suez Canal, named L2 and L3. For the past two decades, *A. taxiformis* is present yearlong at the Israeli coastline with major blooms causing environmental nuisance. Using DNA barcoding, the cryptic lineage 4 (L4) of *A. taxiformis* first reported for the Mediterranean Sea, and previously described for the western Indo-Pacific and Hawaii. Our data indicate a Lessepsian migration route with yet unknown consequences for the local marine ecosystems. Much of *A. taxiformis* invasiveness is attributed to the rich chemistry it produces, specializing in halogenated compounds, mainly brominated, that are sequestered in unique glands found across tissue cells. We explore implications and applications of this invader by seasonal abundance, physiology, reproduction, metabolome, and microbiome diversity.

### **Structure of narwhal tusk studied by X-ray dark field imaging**

Adrian Rodriguez Palomo ([adrian.rodriquez@inano.au.dk](mailto:adrian.rodriquez@inano.au.dk))

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Narwhals are fascinating animals with left-handed spiral tusks with highly anisotropic mechanical properties. We hypothesize that the orientation of the biological nanostructure reflects the spiral macro-structure, which defines the mechanical properties. Using 2D and 3D X-ray imaging techniques we studied its hierarchical structure at multiple length scales and with different contrasts. X-ray scattering, diffraction and fluorescence revealed a complex hierarchical organization of the tusk's building blocks (i.e., mineralized collagen fibres) with a strong anisotropy in a 3D arrangement.

## **SESSION IX: Marine questions / Part V**

### **Biom mineralization of Mantis Shrimp Dactyl Club during Development**

Henrik Birkedal ([hbirkedal@chem.au.dk](mailto:hbirkedal@chem.au.dk))

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Mantis shrimp dactyl clubs have complex biomineralized structures and are reported to form by a die-and-cast process. How the biomineralization process occurs is, however, less understood. Therefore, we study mantis shrimp dactyl clubs collected at specific time points since molting to obtain a time-lapse-series of data on the biominerals. This is achieved by using position resolved synchrotron X-ray diffraction and fluorescence. Furthermore, we combine tomography and diffraction to reveal that the amorphous calcium carbonate in some clubs crystallizes into calcite suggesting that the clubs have a 'design safety factor' built into them. Finally, steps toward mapping the amorphous mineral components in the club will be discussed.

## **Structure and Composition of biomaterials investigated by X-ray Scattering and Fluorescence Tomography**

Ernesto Scoppola ([ernesto.scoppola@mpikg.mpg.de](mailto:ernesto.scoppola@mpikg.mpg.de))

*Max Planck Institute of Colloids and Interfaces, Department of Biomaterials, Potsdam Science Park, Am Mühlenberg 1, 14476 Potsdam OT Golm, Germany*

New imaging methods, based on small angle X-ray scattering (SAXS) and tensor tomography have shown the capability to reconstruct the 3D map of orientation of collagen fibers in trabecular bone and teeth. Recently, we developed a new and fast method to reconstruct 3D maps of the thickness of mineral particles in bone from SAXS data. We have extended this methodology to X-ray Fluorescence (XRF) to reconstruct 3D distribution of specific elements (i.e. Bromine, Zinc) in Limulus Polyphemus cornea cones.

## **The concomitant role of amorphous calcium carbonate and organic molecules in forming colourful sea urchin single crystalline biominerals with convoluted porous structures**

Marie Albéric ([marie.alberic@sorbonne-universite.fr](mailto:marie.alberic@sorbonne-universite.fr))

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Colorful sea urchin spines showing intricate shapes and morphologies grow via the deposition of amorphous calcium carbonate (ACC) that subsequently crystallizes into single-crystalline calcite. Applying the heat-stimulated crystallization of remnant ACC and destruction of intra-crystalline organic molecules of sea urchin spines, we evidenced by HR-XRD, calcite lattice distortions originating in strong atomic interactions and showed by in situ heating SAXS measurements, the evolution of nano-pores, which likely compensate mineral volume shrinkage during ACC crystallization and organics removal.

## POSTER ABSTRACTS

### **A window to diatom bio-silica mineralization**

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Diatoms are microscopic marine algae that exhibit a high degree of control in forming a bio-silica cell wall, in a biomineralization process. In my research, I am looking into a unique biologically controlled silica deposition process, which gives rise to an intricate extension of the cell wall. My primary approach is in-situ cryo-electron tomography, which allows nanoscale investigations of the native state properties inside the cell.

### **Hard X-ray nanoprobe imaging of cultivated coccolithophores**

Daniel Chevrier ([daniel.chevrier@cea.fr](mailto:daniel.chevrier@cea.fr))

*Centre national de la recherche scientifique (CNRS), Cité des énergies 1900, 13108 Saint Paul lez Durance, France*

Coccolithophore microalgae are widespread producers of CaCO<sub>3</sub>-based biominerals (coccoliths). Past production of coccoliths has partly shaped the surface of our planet. Today, their formation and sedimentation play a role in the blue C cycle. How this biomineralization activity will change in future oceans is an open question. Thus, advancing our understanding of coccolith formation is a key barrier to overcome. This work presents hard X-ray nanoprobe measurements of cultivated coccolithophores in varied states of biomineralization and the possibility to measure living cells directly in liquid.

### **Using mineral deposits for breast precancer prognosis**

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We study physiochemical properties of microcalcifications, pathological calcium-containing minerals that form in soft tissues, associated with disease progression. We spatially characterize minerals embedded within tissue sections, especially calcium carbonate and hydrates of calcium oxalate. To correlate crystal properties and malignancy, we measure the mineral crystal phase, chemical composition, particle size and morphology by integrating electron microscopy and vibrational spectroscopy techniques. To obtain the Ca near-edge structure, we will use X-ray fluorescence mapping and Ca K-edge micro XANES.



### **Site-Specific Residual Strains in Calcitic Shells**

Shahrouz Amini ([shahrouz.amini@mpikg.mpg.de](mailto:shahrouz.amini@mpikg.mpg.de))

*Max Planck Institute of Colloids and Interfaces, Department of Biomaterials, Potsdam Science Park, Am Mühlenberg 1, 14476 Potsdam OT Golm, Germany*

Biological ceramics are complex structures that often adapt local properties through gradients in chemistry and architecture to achieve remarkable mechanical performance. Here, by showcasing functional gradients in calcitic shells, we revealed how the distribution of residual strains, a contributory factor to the mechanical performance of biological ceramics, varies across the tissue and how these graded pre-strains contribute to the tissues' mechanical performance. We emphasized the importance of techniques allowing the site-specific analysis of the biological ceramics through high-resolution mapping.

### **Bioinspired Calcium Phosphate Mineralization on Fibrous Chitosan Scaffolds for Bone Regeneration**

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Chitosan fiber scaffolds were functionalized by mineralization with organically modified hydroxyapatite. For this purpose, the scaffolds were embedded in a gelatine gel, serving as a barrier between two liquid reservoirs. These provided calcium and phosphate ions for subsequent electric field-based double migration. In this process, the formation of ormoHAP, which is homogeneously distributed only on the chitosan fiber surfaces and is limited in growth, keeps the scaffold pores open so that bone cells are not prevented from ingrowing. This can improve biological performance by mimicking the bone matrix.

### **Plate-like Guanine Biocrystals Form via Templated Nucleation of Crystal Leaflets on Preassembled Scaffolds**

Zohar Eyal ([zohar.baram@weizmann.ac.il](mailto:zohar.baram@weizmann.ac.il))

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Controlling the morphology of crystalline materials is challenging, as crystals have a strong tendency toward thermodynamically stable structures. Yet, organisms form crystals with distinct morphologies, such as the plate-like guanine crystals produced by many terrestrial and aquatic species for light manipulation. Using cryo-electron tomography of developing zebrafish larvae, we found that guanine crystals form via templated nucleation of thin leaflets on preassembled scaffolds made of 20-nm-thick amyloid fibers. These leaflets then merge and coalesce into a single plate-like crystal.

### **Ca and P-rich intracellular vesicles in coccolithophores and sea urchin embryos**

Rebecca Leghziel ([rebecca.leghziel@weizmann.ac.il](mailto:rebecca.leghziel@weizmann.ac.il))

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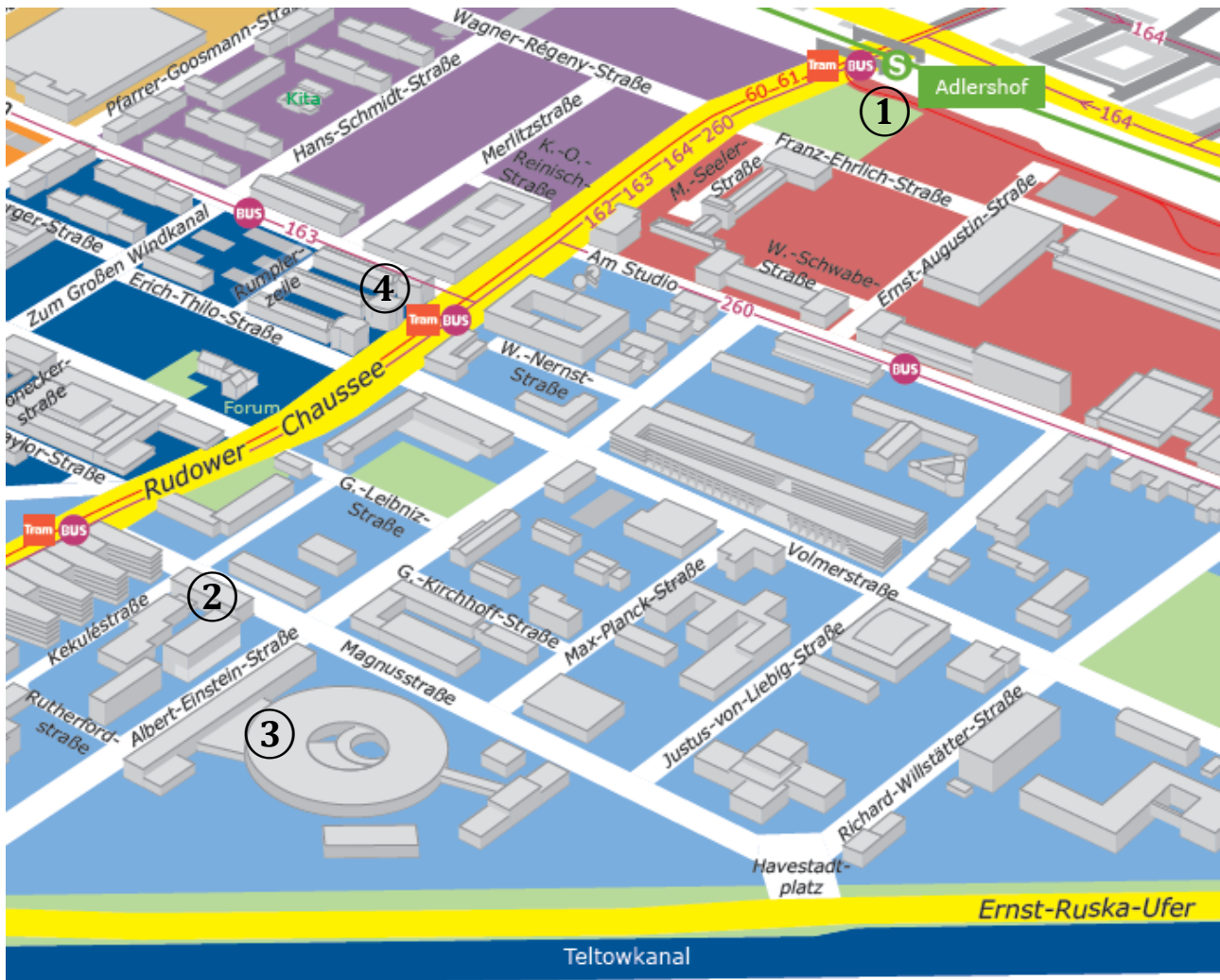
Coccolithophores and sea urchin embryos form morphologically complex calcite crystals. To do so, they must deal with concentrating Ca for the formation of mineralized structures, while maintaining cytosolic concentrations below sub-micromolar range (100-200 nM). Intracellular vesicles containing high concentrations of Ca (1-15 M) and, surprisingly, P appear in coccolithophores and in the primary mesenchymal cells (PMCs) responsible for calcification in sea urchins. Characterization of the Ca-P bodies is key to understand how the organisms concentrate and manipulate Ca intracellularly.

## Campus Map Berlin-Adlershof

Helmholtz-Zentrum Berlin

Albert-Einstein-Straße 15

12489 Berlin



① Train station Adlershof

③ BESSY II Experimental Hall  
Guided Tours / 19 June 2023

② Lecture hall "KINO"  
HKB building 13.10  
Magnusstraße 2

④ Airport hotel Adlershof