ProRat
PromovierendenRat
der TU Bergakademie Freiberg

6th June 2025

BOOK OF ABSTRACTS

9th PhD Conference

RESEARCH DATA: RESPONSIBILITY, ACCOUNTABILITY, SUSTAINABILITY

Contents

1 Welcome Words

As a cherished tradition, we are thrilled to announce the 9th Freiberg PhD Conference, scheduled to take place on the final day of the BHT. This interdisciplinary symposium promises a captivating showcase of oral and poster presentations, providing a window into the captivating and diverse research endeavours undertaken by our university's doctoral candidates.

In this edition, our focus is on raising awareness of how we handle our research data and why it is becoming increasingly important. Our distinguished keynote speakers will present what needs to be considered when backing up and storing data in the long term and which systems are increasingly becoming the standard. They will also look at the ethics of science and discuss what ethical considerations are important and what consequences our research may have.

Do you wish more people were aware of your research and desire to enhance your presentation skills? Are you eager to delve into the research of your peers? If so, we invite you to join us at the 9th Freiberg PhD Conference in 2025! You can contribute by presenting your own research either through an oral presentation or a poster, or simply immerse yourself in the discussions, listening to others and posing questions.

Connect with our PhD students, engage in idea exchange, gain invaluable conference experience, and hone your language proficiency. We eagerly anticipate your participation!

Your PhD Council (ProRat)

2 About Us

We, the PhD Council (PromovierendenRat, ProRat) at TU Bergakademie Freiberg, represent the interests of all PhD candidates at this university. Elected every two years, we are currently in our 7th electoral term. Our work includes supporting networking among PhD candidates in Freiberg and facilitating connections with PhD student representatives from other universities in Saxony, Saxony-Anhalt, and Thuringia (VMPV, LAMS) as well as Germany (Bundesverband Promovierende). We also represent PhD candidates in rectorate commissions and participate in senate and faculty councils. Additionally, we provide statements on higher education policies, such as amendments to SächsHSG and WissZeitVG, and offer support and advice to PhD candidates with individual questions or problems.

Do not hesistate to contact us, if you have any questions or ideas or if you want to join ProRat as a freelancer. Contact `info@prorat.tu-freiberg.de`!

Visit our website

Subscribe to our newsletter

Fig. 1: Our six currently elected members of the PhD council (from left to right): Hanna Böhme, Debora Pötschke (speaker), Elisabeth Heise, Sarah Kuß, Bernhard Berger, Hagen Fiebig (chairman). (Image: Alexander Weiß)

3 Programme

GREETING		
9:00 – 9:10	Hagen Fiebig	

KEYNOTE PRESENTATION CHAIR: Hagen Fiebig		
9:10 – 10:00	Dr. Marco Krüger	**Why we need (good) Research Ethics**

ORAL PRESENTATIONS: SESSION 1 – SUSTAINABLE MINING CHAIR: Hagen Fiebig		
10:00 – 10:20	Akuba Bezeba Yalley	Development of safe and sustainable mining methods for artisanal and small-scale gold mining operations with alluvial and hard rock potentials
10:20 – 10:40	Sarah Kuß	Establishing reductive, microbial processes for waste water treatment and value recovery

POSTER SESSION 1 AND COFFEE BREAK 10:40 – 11:45		
A1	Deepak Varma Thota	Investigation of Hydrogen Flame Effects and Long-Term Aging in a Hydrogen Atmosphere on Additive Manufactured Ceramics
A2	Klara Sander	Characterisation of Biopolymers using ultrahigh-resolution Mass Spectrometry
A3	Sophie Manke	Characterization of microalgae isolated from biological soil crusts on a heavy metal contaminated mining deposit
A4	Mareike Weigel	Development and Application of New Sol-Gel Systems: From Biofouling Reduction to Sensor Applications
A5	Lena Bonitz	Stability of polyhalite in salt solutions at 25 °C

A6	Hagen Fiebig	Stability of Selected Magnesium Carbonate Phases in $MgCl_2$ Solutions: Data for Rock Salt Based Nuclear Waste Repositories
A7	Enver Felix Loayza Mora	Droplet based microfluidics and miniaturization at high throughput level to screening heterologous secondary metabolites in microbes: A critical review
A8	Samaneh Mollashahi	Turning invasive plants into energy: Assessing biogas production from invasive species through LCA
A9	Anne Seidel	Sustainable Dipeptide Synthesis for Biocompatible Applications
A10	Willi Max Leopold	From Molecules to Materials: Tuning Sol-Gel Coatings through Experimental Design

ORAL PRESENTATIONS: SESSION 2 – GEOTECHNOLOGY CHAIR: Sarah Kuß		
11:45 – 12:05	Duncan Maina	The effect of the intermediate principal stress for dimensioning in room and pillar mining
12:05 – 12:25	M G Muntasir Shehab	Physics-based machine learning models for predicting saturated and unsaturated hydraulic conductivity of bentonite with global sensitivity analysis
12:25 – 12:45	Reza Mahmoudi Kouhi	A coupled hydro-mechanical model using Modified Cam-Clay for predicting swelling behavior of clay–sulfate rocks

BREAK 12:45 – 13:45		

KEYNOTE PRESENTATION CHAIR: Hagen Fiebig		
13:45 – 14:30	Dr. Steffen Neumann	**Modern RDM in Chemistry**

ORAL PRESENTATIONS: SESSION 3 – MATERIAL SCIENCE I CHAIR: Bernhard Berger		
14:30 – 14:50	Shuvam Gupta	3D characterization of rare earth in iron ore
14:50 – 15:10	Mohammed Shakeer Khan	Investigating the Empirical Relationship Between Amine Flow and Sand Core Curing in Polyurethane Cold Box System

COFFEE BREAK 15:10 – 15:35

ORAL PRESENTATIONS: SESSION 4 – MATERIAL SCIENCE II CHAIR: Elisabeth Heise		
15:35 – 15:55	Sahra Homaee	Optimizing Wet Carbonation of Wollastonite for Accelerated CO_2 Capture and Application in the Cement Industry
15:55 – 16:15	Fritz Raithel	Development of a method for creating standardised load profiles for cooling buildings

CLOSING REMARKS	
16:15 – 16:30	Elisabeth Heise

AFTER CONFERENCE BBQ
(AWNING, NEUE MENSA)
16:30 – open end

4 Keynotes

Dr. Marco Krüger

Universität Tübingen | International Center for Ethics in the Sciences and Humanities (IZEW)

marco.krueger@izew.uni-tuebingen.de

Topic

Warum wir (gute) Forschungsethik brauchen / Why we need (good) Research Ethics

Dr. Steffen Neumann

NFDI4Chem (Nationale ForschungsDatenInfrastruktur) Lead of TA 4
Leibniz-Institute for Plant Biochemistry (IPB), Halle (Saale)

steffen.neumann@ipb-halle.de

Topic

Modern RDM in Chemistry

5 Abstracts

5.1 Oral abstracts

Development of safe and sustainable mining methods for artisanal and small-scale gold mining operations with alluvial and hard rock potentials

Akuba Bezeba Yalley

Department of Mining Engineering, University of Mines and Technology, P.O. Box 237, Tarkwa, Ghana

abyalley@umat.edu.gh

Abstract

Artisanal and small-scale gold mining (ASGM) operations are known to contribute significantly towards rural economic development. The operations which are widespread in about 80 countries across Africa, Asia, Oceania, Central and South America have the potentials to alleviate poverty, create employment opportunities, generate income and produce large quantities of the precious mineral gold. In spite of all these potentials, the sector is associated with high levels of environmental degradation, health and safety threats and low productivity that threaten the sustainability of the sector. These challenges have been linked to the use of inappropriate mining methods for the various deposit types exploited. In mining engineering principle, the selection of a suitable mining method for a particular ore deposit is critical for the environmental, safety and economic sustainability of a mining project. However, little attention has been given to the subject of development of sustainable mining methods for ASGM operations. This study seeks to fill the gap in science by developing safe and sustainable mining methods for ASGM operations with alluvial and hard rock potentials. These particular deposit type has been chosen because it the most exploited deposit type by ASGM miners. The methods used include literature review of the occurrence of this deposit type. Field visits were made to 3 ASGM sites in Ghana exploiting this deposit types and the challenges the miners have with the mining methods they are using. The Geovia Surpac software version 2024 was used in the design of the mining methods for both manual and mechanised operations. Proposed work schedules, equipment requirement and labour requirement have been provided as a guideline for the miners. The developed mining methods will guide the miners to carry out their operations in a safe and sustainable manner. It is therefore recommended ASGM operations engage mining engineering and allied professionals to ensure effective implementation of the developed mining method.

Establishing reductive, microbial processes for waste water treatment and value recovery

Sarah Kuß*, Marika Hofmann, Sabrina Hedrich

Institute of Biosciences, TU Bergakademie Freiberg

sarah.kuss@bio.tu-freiberg.de

Abstract

In the Ore mountains mining region and its surrounding areas, there are numerous abandoned mines and several thousand mine dumps. Some of these dumps still contain large quantities of strategic and critical metals, but at the same time pose a threat to the environment through the uncontrolled release of harmful species (metals, metalloids, sulfate). Systems utilizing sulfate- and iron-reducing microorganisms represent a promising biotechnological approach for the treatment of metal- and sulfate-laden waters, facilitating both, the de contamination of the environment and the recovery of valuable resources. To establish and optimize the respective biological water treatment system, microorganisms were enriched from samples taken at the Reiche Zeche mine in Freiberg (Germany) and "Roter Graben", a stream accumulating metal-rich process waters from the mine and other local industries. Anaerobic enrichment cultures were set up under various conditions, including media for iron- and sulfate-reducing microorganisms with different substrates, pH-values and temperatures. First results indicate the presence of sulfate-reducing bacteria in Postgate B medium.

In further studies, genes involved in the reduction of sulfate and ferric iron will be identified in order to better understand and influence the reactions taking place in the organism. The results will be transferred to bioreactor studies for process development, which will allow targeted control of the complex processes and investigation of different parameters for efficient extraction of valuable metals and separation of pollutants.

The effect of the intermediate principal stress for dimensioning in room and pillar mining

Duncan Maina

Institute of Geotechnics, TU Bergakademie Freiberg

Duncan.Maina@doktorand.tu-freiberg.de

Abstract

The room and pillar mining method is widely used mining technology to ensure stability and low environmental impact. Existing pillar and drift design methods are based on classical failure criteria, which do not consider the intermediate principal stress component. Based on the detailed analysis of existing true triaxial failure criteria, an extended Hoek-Brown criterion (called EHB) is proposed as an advanced alternative for drift and pillar design. The EHB model is implemented into the explicit finite difference code FLAC3D and several exemplary mine pillar and drift models were created. The corresponding numerical simulations comparing EHB and classical HB model results show that the intermediate principal stress component significantly influences pillar strength, factor-of-safety, extraction ratio, stress concentration factor, and volume (extent) of the excavation disturbed zone. These results lead to improved predictions of failure mechanisms and provide a reliable and efficient framework for mine design.

Physics-based machine learning models for predicting saturated and unsaturated hydraulic conductivity of bentonite with global sensitivity analysis

M G Muntasir Shehab*, Reza Taherdangkoo, Christoph Butscher

Institute of Geotechnics, TU Bergakademie Freiberg

M-G-Muntasir.Shehab@student.tu-freiberg.de

Abstract

Bentonite is proposed as a buffer material for the geotechnical barrier in high-level radioactive waste repositories. Accurate prediction of saturated and unsaturated hydraulic conductivity of bentonite is critical for assessing water flow and saturation time in such repositories. This study develops a data-driven machine learning (ML) model to predict saturated hydraulic conductivity and a physics-based ML model to predict unsaturated hydraulic conductivity of bentonite. For the saturated hydraulic conductivity prediction, a dataset of 215 experimental measurements was compiled, incorporating key soil properties such as montmorillonite content, specific gravity, plasticity index, initial water content, dry density, and temperature. The predicted saturated hydraulic conductivity values were then used as input to the physics-based ML model for predicting unsaturated hydraulic conductivity. Additionally, the physics-based ML model was trained using a combination of 311 experimental data points and 920 synthetic data points generated using the Van Genuchten model. The experimental dataset includes specific gravity, montmorillonite content, initial dry density, initial water content, initial void ratio, plasticity index, suction, and volumetric water content. The synthetic data includes suction, volumetric water content, and unsaturated hydraulic conductivity. The CatBoost and XGBoost algorithms were used to train the ML models, and the Whale Optimization Algorithm was applied for hyperparameter tuning. The trained ML models show good performance in predicting both saturated and unsaturated hydraulic conductivity of bentonite based on key soil parameters.

A coupled hydro-mechanical model using Modified Cam-Clay for predicting swelling behavior of clay–sulfate rocks

Reza Mahmoudi Kouhi*, Reza Taherdangkoo, Thomas Nagel, Faramarz Doulati Ardejani, Christoph Butscher

Institute of Geotechnics, TU Bergakademie Freiberg

Reza.Mahmoudi-Kouhi@doktorand.tu-freiberg.de

Abstract

Swelling of clay–sulfate rocks is a major concern in geotechnical engineering because of the complex interaction between hydraulic processes and mechanical deformation. In the historic town of Staufen (southwest Germany), geothermal drillings into anhydrite-bearing formations triggered severe ground heave, resulting in serious damage to more than 250 houses. This event highlighted the importance of understanding swelling processes in clay–sulfate rocks. In this study, a coupled hydro-mechanical model was developed to investigate the swelling problem at the city of Staufen, located in south-west Germany. The model employs the Modified Cam-Clay (MCC) for mechanical processes coupled with Richards' equation to describe fluid flow within porous media. The model takes into account spatial heterogeneity of material properties, namely Young's modulus and permeability within the swelling layer, to represent depth-dependent variations observed at the study site. Finally, the model is calibrated using data from 2009 to 2011, employing a Grey Wolf Optimization algorithm to reduce the difference between simulated and measured ground heave data. The results show that applying a complex elasto-plastic model with consideration of heterogeneity can accurately reproduce the mechanical deformations observed at Staufen. The model predicts the heave data until the end of 2024 with sufficient degree of accuracy, although these data were not used during the calibration process.

3D characterization of rare earth in iron ore

Shuvam Gupta

Helmholtz Institute Freiberg, TU Bergakademie Freiberg

shuvamgupta56@gmail.com

Abstract

The recently developed Mounted Single Particle Characterisation and Mineralogical Analyses (MSPaCMAn) workflow enables the quantification of small rare earth mineral (REM) grains within particulate iron ore samples. In these samples, REMs commonly occur as minute inclusions, posing significant challenges for X-ray computed tomography (CT) due to partial volume and blurring effects—particularly when grain sizes approach the voxel resolution. The enhanced MSPaCMAn workflow addresses these limitations by incorporating additional steps that simultaneously analyse grey values and geometrical features of REMs and their host minerals. This refinement also facilitates detailed characterisation of particle surfaces. The reliability of the MSPaCMAn results was validated using scanning electron microscopy-based automated mineralogy and X-ray powder diffraction. Overall, the study advances the accurate and reproducible mineralogical quantification of processed particulate samples through 3D X-ray imaging.

Investigating the Empirical Relationship Between Amine Flow and Sand Core Curing in Polyurethane Cold Box System

Mohammed Shakeer Khan

Foundry Institute, TU Bergakademie Freiberg

Mohammed.shakeer-khan@gi.tu-freiberg.de

Abstract

Polyurethane Cold Box (PUCB) systems are widely used for manufacturing sand cores in foundry applications due to their efficiency and cost-effectiveness. Despite their industrial relevance, a significant knowledge gap persists in understanding how amine vapor—the catalyst used for curing—flows through the porous sand structure and interacts with the binder to achieve complete and uniform curing. This lack of insight stems from the absence of reliable quantitative methods to track amine flow dynamics and curing progression within the core.

To address this challenge, this study employs a novel ultrasonic sensor-based measurement technique to investigate the relationship between amine flow and core curing behavior. Experimental trials are conducted on sand cores produced using a universal coremaking machine, with and without binder, to characterize amine transport mechanisms and quantify in-flow vs. out-flow rates. A detailed amine mass balance is developed to determine the purging efficiency and curing progression over time. Key process parameters—including core length, amine concentration, and total mass—are systematically varied to analyze their impact on curing rate and completeness.

The results reveal a strong correlation between amine concentration and curing duration, demonstrating their combined effect on localized hardening rates and overall curing quality. Empirical models are derived to establish functional relationships between amine flow parameters and curing behavior, providing valuable insight for optimizing process control and minimizing defects such as incomplete curing or weak core spots.

This study offers a pioneering approach to visualizing and quantifying core curing dynamics, contributing to enhanced quality assurance, reduced cycle times, and more sustainable amine usage in PUCB-based sand core manufacturing.

References:
1. M. Holtzer, A. Kmita, Mold and Core Sands in Metalcasting: Chemistry and Ecology Sustainable Development (Springer, Cham, 2020), p.186. https://doi.org/10.1007/978-3-030-53210-9
2. Khan, M. S., Mrowka, N. M., Sablowski, J., Asghar, M. T., Kupsch, C., and Szucki, M.: Investigations of the Cold Box Core Curing Stage Using an Augmented Simulation Approach, Inter Metalcast, https://doi.org/10.1007/s40962-024-01445-y, 2024.
3. Khan, M. S. and Szucki, M.: Numerical and Experimental Analysis of Amine Flow in Foundry Sand Cores, in: Proceedings of the 10th World Congress on Mechanical, Chemical, and Material Engineering (MCM'24), The 10th World Congress on Mechanical, Chemical, and Material Engineering, Barcelona, Spain, https://doi.org/10.11159/htff24.253, 2024.
4. Source: Jakob Sablowski, Muhammad Talal Asghar, Mohammed Shakeer Khan, Michal Szucki,

Christian Kupsch.Ultrasonic time of flight measurements for inline gas analysis and process monitoring in the phenolic urethane cold box process.

Measurement, Sensor and Embedded Systems Laboratory, TU Bergakademie Freiberg, Freiberg, 09599, Germany
Foundry Institute, TU Bergakademie Freiberg, Freiberg, 09599, Germany. (accepted)

Optimizing Wet Carbonation of Wollastonite for Accelerated CO_2 Capture and Application in the Cement Industry

Sahra Homaee*, Martin Rudolph

Helmholtz Institute Freiberg for Resource Technology (HIF), Dresden University of Technology

s.homaee@hzdri.de

Abstract

The steady rise in carbon dioxide (CO_2) emissions from fossil fuel combustion as well as from Cement production, remains a major environmental concern, prompting urgent action to mitigate climate change. In support of the Paris Agreement's goal to limit global temperature rise to below 2 °C – ideally 1,5 °C – there is a growing emphasis on carbon capture strategies that not only reduce emissions but also promote circular carbon use in industrial processes. Among emerging approaches, wet mineral carbonation offers a promising pathway for CO_2 sequestration, especially within the cement industry. The use of carbonated silicate-based materials as Supplementary Cementitious Materials (SCMs) provides a dual benefit: reducing emissions while recycling CO_2 into valuable construction materials. Although wet carbonation is known for its rapid reaction kinetics in aqueous media, further understanding of its reaction mechanisms is essential for optimizing performance.

This study investigates the optimization of wollastonite carbonation under ambient conditions (non-pressurized reactor) using a full factorial Design of Experiments (DOE) approach. The factors studied and optimized include temperature, solid-to-liquid ratio (S/L), CO_2 flow rate, and stirring speed (RPM). The optimal conditions identified were 90 °C, 10 % S/L, a CO_2 flow rate of 700 mL min^{-1}, and 900 RPM. Under these conditions, more than 50 % of the theoretical carbonation potential of the studied wollastonite was achieved.

Development of a method for creating standardised load profiles for cooling buildings

Fritz Raithel

Professorship for Technical Thermodynamics, TU Bergakademie Freiberg

fritz.raithel@ttd.tu-freiberg.de

Abstract

Cooling buildings is becoming increasingly important for adapting to climate change. The aim of the PhD-thesis is to develop a method for creating standard load profiles (SLP) for building cooling. SLP represent the statistic average for specific consumer groups. They are necessary for network and capacity planning, load management and simulations of energy grids. While SLP based forecasts show inaccuracies for individual consumers they become increasingly precise with rising consumer numbers. The cooling demand is defined as the sum of heat gains and losses via the building shell leading to an increase the indoor temperature above the defined maximum temperature. SLPs will be derived from the building specific cooling demand for Saxony. This will be determined with the help of GIS and the calculation principles and boundary conditions defined in DIN 18599 and validated with representative measurements on and in selected buildings.

5.2 Poster abstracts

A1 Investigation of Hydrogen Flame Effects and Long-Term Aging in a Hydrogen Atmosphere on Additive Manufactured Ceramics

Deepak Varma Thota*, Sven Eckart, Florian Kerber, Hartmut Krause, Christos Aneziris

Professorship for Gas and Heat Technology, Institute of Thermal Engineering, TU Bergakademie Freiberg

Deepak-Varma.Thota@iwtt.tu-freiberg.de

Abstract

As hydrogen emerges as a sustainable alternative to fossil fuels, understanding its interaction with high-temperature materials is critical for advancing combustion technologies. This study investigates the effects of hydrogen flames and long-term hydrogen exposure on additively manufactured ceramics (alumina and spinel) to assess their viability in applications such as gas turbines and internal combustion engines. Two experimental approaches are used to study hydrogen flame interactions and material durability: Flame-wall interaction (FWI) tests using a custom-designed hydrogen burner to quantify quenching distances and characterize flame dynamics under conditions mimicking closed combustion geometries. Temperature profiles are mapped via laser-induced fluorescence (LIF) by analyzing OH radical behavior. Long-term aging tests [2] are conducted in a tube furnace at 1500 °C for up to 600 hours under hydrogen and natural gas atmospheres to evaluate thermal stability and corrosion resistance. Post-test analyses of the specimens included mass loss quantification and surface degradation assessment using laser-induced plasma spectroscopy (LIPS) microscopy.

A2 Characterisation of Biopolymers using ultrahigh-resolution Mass Spectrometry

Klara Sander*, Jan Zuber, Erica Brendler, Carla Vogt

Institute of Analytical Chemistry, TU Bergakademie Freiberg

klara.sander@chemie.tu-freiberg.de

Abstract

Plant cell walls consist primarily of cellulose, hemicellulose and lignin, forming lignocellulosic biomass - a renewable and abundant resource, which offers a wide range of applications and therefore is discussed as renewable alternative to fossil resources in various fields of interest, for example for chemical and pharmaceutical industries. To effectively utilise celluloses and hemicelluloses, understanding their structure is essential. However, their analysis can be challenging due to the insolubility of celluloses and the structural variability of hemicelluloses. High-resolution analytical techniques like high-resolution mass spectrometry (HRMS), including Fourier-transform ion cyclotron resonance mass spectrometry (FT-ICR-MS), combined with laser desorption ionisation sources, offer promising solutions for analysing these complex biopolymers.

In this work, new analysis routines for the characterisation of hemicelluloses and celluloses were developed, using graphite-assisted laser desorption/ionization (GALDI) combined with FT-ICR-MS, offering an alternative to existing methods utilizing photoactive organic matrices. These methods permitted the direct analysis of solid biopolymer samples in both positive and negative ionization modes. For example, it was possible to detect structurally different oligomer series in a beechwood xylan sample, indicating a substitution of the xylose chain with 4-O-methyl glucuronic acid and a partial acetylation of the main chain. Whereas the detection of different oligomer series in cellulose samples suggests the elimination of multiple water molecules during ionisation. Additional structural insights were gained through NMR, IR spectroscopy and tandem MS. It is hoped that these methods and the generated results will contribute to a deeper understanding of the structural peculiarities of biomass and thus will help to establish it as alternative to fossil resources.

A3 Characterization of microalgae isolated from biological soil crusts on a heavy metal contaminated mining deposit

Sophie Manke

Institute of Biosciences, TU Bergakademie Freiberg

sophie.manke@ioez.tu-freiberg.de

Abstract

One of the largest mining deposits in Freiberg is the Davidschachthalde, which was built from 1944 to 1969 from deposits of flotation residues. These deposited flotation residues consisted primarily of unusable, waste rock with high concentrations of arsenic, lead and cadmium. As a result, heavily contaminated soils with litle vegetation developed. These toxic elements still leach today into groundwater and surface water, including the Freiberger Mulde. The tailing was partly covered with other waste material, like construction waste. In those areas, pioneer plants like grasses and birches developed. Nevertheless, some areas are still vegetation-free or accommodate only sparse vegetation and prone to erosion and a potential source for contaminated water and dust even after more than 50 years without mining activities. One possible method to secure the tailing could be the initiation of biological soil crusts (biocrusts). Biocrusts are composed of algae, bacteria, fungi, lichens and mosses and form on the soil surface. They conduct important ecological functions, like soil stabilization, reduction of erosion, increasing the nutrient input and alteration of water retention. Overall, biocrusts can improve the soil conditions for the colonization of higher plants. They can reduce the development of contaminated dust. The emission of contaminated water is also reduced by absorption of rainwater and transpiration through the biomass at the soil surface. The aim of the work is to investigate the possible initiation of biocrusts by applying algae biomass on the surface soil. For this purpose, samples of naturally-developed biocrusts were first taken from the vegetation-free area of the tailing. The algae were isolated and will be ecophysiologically characterized with special regard to their heavy metal tolerance. Alga species will be selected as potential candidates to initiate biocrust formation based on their heavy metal tolerance, their growth rate and their ability to secrete mucilage, which 'glues' the soil particles together and thus, stabilize the soil surface.

A4 Development and Application of New Sol-Gel Systems: From Biofouling Reduction to Sensor Applications

Mareike Weigel[a,b]*, Amy Albrecht[c], Jan Beyer[c], Lukas Oppelt[d], Konstantin Kraushaar[a,b] and Edwin Kroke[a,b]

[a] Institute of Inorganic Chemistry, Silicon Chemistry & Chemical Materials Science, TUBAF, Freiberg, Germany
[b] Centre for efficient high-temperature material conversion (ZeHS), TUBAF, Freiberg, Germany
[c] Institute of Applied Physics, Spectroscopy working group, TUBAF, Freiberg, Germany
[d] Institute of Thermal Engineering, Technical Thermodynamics, TUBAF, Freiberg, Germany

mareike.weigel@chemie.tu-freiberg.de

Abstract

Two different sol-gel systems based on organofunctional alkoxysilanes and titanium alkoxides were developed as part of this work.[1,2] The sol-gel method makes it possible to convert liquid precursors such as alkoxysilanes into solid, cross-linked structures through a controlled sequence of hydrolysis and condensation reactions. The choice of precursors leads to significant differences in the material properties of the two systems, which opens up a wide range of possible applications. The application of the developed systems was tested both in cooperation with industrial partners and across faculties at our university. One of the formulations, which was modified with the biopolymer chitosan, is suitable for coating boat propellers and heat exchangers to reduce biofouling, for example.[3] The second formulation was used to embed nanodiamonds in order to fix them homogeneously to an optical fibre and thus enable their use as a magnetic field-sensitive sensor.[4] Due to the special geometry of the glass fiber, greater flexibility is required, which is why dimethyldiethoxysilane was integrated into the sol-gel formulation.

[1] E. Kroke, K. Kraushaar, M. Weigel, Patent DE102023118077A1, 2025.
[2] E. Kroke, K. Kraushaar, M. Weigel, M. Bös, A. Seidel, Patent DE102023116864A1, 2025.
[3] M. Bös, L. Gabler, W. M. Leopold, M. Steudel, M. Weigel, K. Kraushaar, Gels, 2024, 10, 1–37.
[4] A. Albrecht, J. Beyer, M. Weigel, K. Kraushaar, to be submitted.

A5 Stability of polyhalite in salt solutions at 25 °C

Lena Bonitz

Institute of Inorganic Chemistry, TU Bergakademie Freiberg

Lena.Bonitz@student.tu-freiberg.de

Abstract

Polyhalite is a triple salt hydrate found in saline formations, which are being considered as potential radioactive waste repositories. Understanding the composition of solutions that may develop upon contact with the minerals of surrounding salt rocks is critical for assessing radionuclide interactions in scenarios involving solution inflow.

This study aimed to initiate experimental investigations into the stability field of polyhalite, addressing discrepancies in the literature and model descriptions (HMW and THEREDA, Figure 2). Solution-solid mixtures were prepared for long-term equilibration, with initial solution concentrations corresponding to points 1–12 in Figure 2.

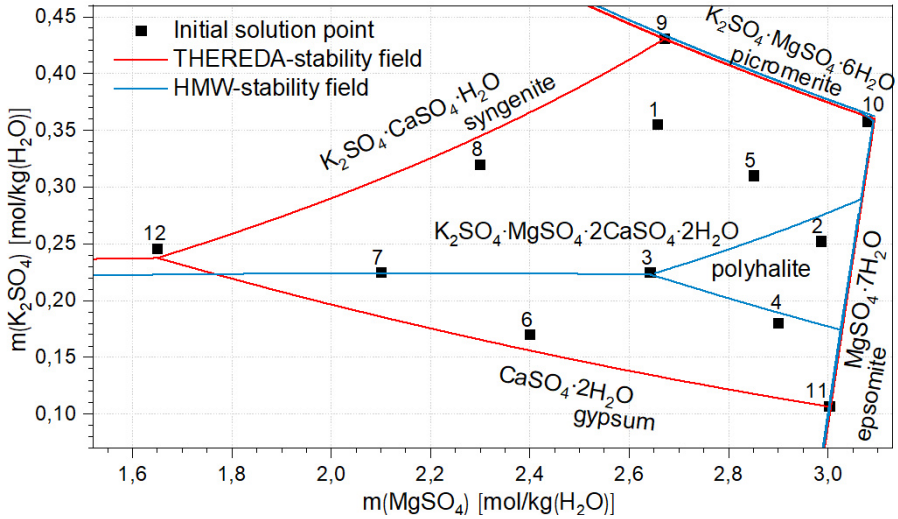

Fig. 2: Polyhalite stability fields in the system K^+, Mg^{2+}, Ca^{2+}, SO_4^{2-} - H_2O at 25 °C according to THEREDA and HMW in projection onto the K_2SO_4-$MgSO_4$-surface with the the 12 initial solutions from this investigation.

The experimental preparation included the synthesis and characterization of initial solid phases. Various calcium sulfate containing solids: hemihydrate, gypsum, syngenite, and polyhalite, were added to these 12 solutions resulting in 65 solution-solid mixtures, and changes in the solid phase composition were analyzed using Raman spectroscopy. Raman analyses demonstrated transformations of the initial phases syngenite, gypsum, and . For all three Syngenite formed at higher K_2SO_4 concentrations, while

gypsum predominated at lower concentrations. Polyhalite formation was observed in one sample with as the initial solid, though no changes were detected in the samples with polyhalite as initial phase during the study period (up to 168 days).

Since different solid phases are still present in identical solution comositions, equilibrium has not yet been achieved, but ongoing efforts aim to determine the polyhalite stability field for the first time at 25 °C in the quaternary system.

A6 Stability of Selected Magnesium Carbonate Phases in $MgCl_2$ Solutions: Data for Rock Salt Based Nuclear Waste Repositories

Hagen Fiebig

Institute of Inorganic Chemistry, TU Bergakademie Freiberg

hagen.fiebig@chemie.tu-freiberg.de

Abstract

Understanding solid-solution equilibria among host rock components, saline solutions, deposited material, and geotechnical barriers is essential for the safety assessment of radioactive waste repositories in rock salt formations. Carbonate equilibria, influenced by CO_2, play a critical role. In this study, magnesium carbonate phases – magnesite ($MgCO_3$), nesquehonite ($MgCO_3 \cdot 3\,H_2O$), hydromagnesite ($Mg_5(CO_3)_4(OH)_2 \cdot 4\,H_2O$), dypingite ($Mg_5(CO_3)_4(OH)_2 \cdot 5\,H_2O$), and chlorartinite ($Mg_2(CO_3)Cl(OH) \cdot x\,H_2O$) – were synthesized and characterized using PXRD, SEM, Raman spectroscopy, and TG-DSC. Phase stability was investigated by suspending the solids in $MgCl_2$ solutions of varying concentrations at 25 °C over extended periods of time. Nesquehonite was unstable, converting to dypingite or chlorartinite depending on $MgCl_2$ concentration and the presence of MgO. Dypingite exhibited metastability, transforming into chlorartinite at higher salinities. Hydromagnesite and magnesite remained stable under all investigated conditions. These findings provide essential baseline data on magnesium carbonate behavior in saline environments. Future work will include stability studies with detailed monitoring of solution compositions, CO_2 partial pressure, and solid components near equilibrium to derive thermodynamic data in the system $Mg(OH)_2$-$MgCl_2$-CO_2-H_2O.

A7 Droplet based microfluidics and miniaturization at high throughput level to screening heterologous secondary metabolites in microbes: A critical review

Enver Felix Loayza Mora

Institute for Nanoscale and Biobased Materials, TU Bergakademie Freiberg

enverloayza@hotmail.com

Abstract

Droplet based microfluidics and automation are important technology to support bio-process and screening during the last years. Main objective of this review is to describe the current technology in monitoring secreting microbes at scale down level. During this study, questions and challenges are shown with relation to this approach specifically in droplet based microfluidics as well as in miniaturized platforms focused on screening of certain metabolites. Relevant challenges to both technologies are described in this article from a technical overview, those that are associated with the control of secondary metabolites as well as growth parameters during microbe cultivation with focus in *Y. lipolidica*, *S. lividians* and *C. glutamicum*. In order to achieve the objective, six studies highlighted on production of metabolites as polyphenols are discussed, as well as the relevancy of analytical methods that are associated with verify development of heterologous micro-organisms during bio process.

A8 Turning invasive plants into energy: Assessing biogas production from invasive species through LCA

Samaneh Mollashahi

Institute of Thermal Engineering, Professorship for Gas and Heat Technology, TU Bergakademie Freiberg

Samaneh.Mollashahi@doktorand.tu-freiberg.de

Abstract

The increasing proliferation of invasive plant species, combined with the partly inadequate management of agricultural residues, poses a serious threat to biodiversity, ecosystem stability, and, consequently, human well-being.

Against this backdrop, the development of efficient and environmentally valorisation technologies is gaining growing importance. Anaerobic digestion (AD) represents an established method for converting organic substrates into biogas and offers promising approaches for addressing these challenges. In the present study, the biogas potential of selected invasive plant species was investigated through batch anaerobic digestion experiments, and their specific methane yields were quantified. Additionally, a method to reduce the duration of batch tests was introduced.

To comprehensively assess the environmental impacts of the energy conversion processes, a life cycle assessment (LCA) was conducted comparing two biomass conversion pathways: the Integrated Generation of Solid Fuel and Biogas from Biomass (IFBB) and conventional anaerobic digestion. The LCA followed a cradle-to-grave approach, encompassing all stages from biomass collection and processing to final energy conversion. The results demonstrate the significant energetic potential of neophytic biomass for biogas production. Furthermore, the LCA identified key emission sources: in AD, methane leakage due to system inefficiencies was found the primary contributor, while not taking into account the performance of the neophytic plants were in a comparable amount. Whereas in the IFBB process, the highest emissions resulted from energy-intensive steps such as pressing, pelletizing, cooling, and drying. These findings contribute to process optimization and provide a scientific basis for selecting resource-efficient technologies for sustainable energy production from biomass.

A9 Sustainable Dipeptide Synthesis for Biocompatible Applications

Anne Seidel*, Jörg Wagler, Edwin Kroke

Institute of Inorganic Chemistry, TU Bergakademie Freiberg

anne.seidel@chemie.tu-freiberg.de

Abstract

Condensation of amino acids via formation of amide groups yields peptides. As two different amino acids (AS1 and AS2) may form four different dipeptides, selective technical production requires the use of protective groups, i.e. time-consuming and costly syntheses via numerous steps.[1] Based on anions of α-AS, which are suitable ligands for Si coordination chemistry,[2,3] a silicon-templated protecting group-free synthesis of dipeptides was developed. Reactions of unprotected amino acids and silanes afford complexes that contain dipeptides in Si-bound form, wherefrom the dipeptide can be cleaved off and isolated.[4,5] The absence of protective groups reduces the number of synthesis steps and reagents, which makes the route more efficient and environmentally friendly. The process is promising for the production of products such as drug carriers, nutrition components (e.g. artificial sweeteners) or building blocks for peptide nanotechnology.[6] Besides, dipeptides are biocompatible and biodegradable.[7]

[1] Hattori, T., Yamamoto, H. J. Am. Chem. Soc. 2022, 144, 1758–1765. doi: 10.1021/jacs.1c11260.
[2] Seidel, A. et al. Molecules 2023, 28, 7816. doi: 10.3390/molecules28237816.
[3] Seidel, A., Wagler, J. Molecules 2025, 30, 834. doi: 10.3390/molecules30040834.
[4] Kowalke, J., Brendler, E., Wagler, J. J. Organomet. Chem. 2021, 956, 122126. doi: 10.1016/j.jorganchem.2021.122126.
[5] Seidel, A., Wagler, J., Kroke, E. DE 10 2024 137 468.3, 2024.
[6] Gong, X. et al. Mater. Sci. Eng. C 2015, 58, 478–486. doi: 10.1016/j.msec.2015.08.059.
[7] Xing, S. et al. Biomacromolecules 2017, 18, 3514–3523. doi: 10.1021/acs.biomac.7b00787.

A10 From Molecules to Materials: Tuning Sol-Gel Coatings through Experimental Design

Willi Max Leopold*, Konstantin Kraushaar, Edwin Kroke

Institute of Inorganic Chemistry, TU Bergakademie Freiberg

Willi-Max.Leopold@chemie.tu-freiberg.de

Abstract

The sol-gel process offers versatile applications in materials science, but its complexity requires systematic optimisation to improve both synthesis and application conditions.[1,2] This study uses Design of Experiments (DoE) to investigate the influence of precursors, catalysts and synthesis routes on the properties of the coatings. Key factors include variations in silane precursors (e.g. methyltriethoxysilane, 3-glycidylpropyltriethoxysilane, tetraethoxysilane), catalyst types (e.g. acetic acid, phosphoric acid, hydrochloric acid) and hardeners (e.g. tetra-n-butyl orthotitanate, zirconium(IV) propoxide, hafnium(IV) n-butoxide).[3,4] Target properties such as processability, coating durability and mechanical performance are systematically analysed. In addition, the effects of fillers, drying conditions and sol preparation methods are investigated. Through the use of statistical methods, this research not only deepens the understanding of the sol-gel process, but also provides a robust framework for optimising material properties, making it highly relevant for industrial and functional applications.[5]

[1] M. Bös, L. Gabler, W. M. Leopold, M. Steudel, M. Weigel, K. Kraushaar, Gels, 2024, 10, 1–37.
[2] C. J. Brinker, G. W. Scherer, Sol-gel science, The physics and chemistry of sol-gel processing, Acad. Press: Boston, 1990.
[3] E. Kroke, K. Kraushaar, F. Gellrich, Patent DE102019110519A1, 2020.
[4] V. Moutarlier, B. Neveu, M. P. Gigandet, Surf. Coat. Technol., 2008, 202, 2052–2058.
[5] A. Rössler, Design of experiment for coatings, European coatings library, Vincentz: Hannover, 2014.

9th PhD Conference 2025
BOOK OF ABSTRACTS

Publisher, Editorial and Design:

PromovierendenRat
TU Bergakademie Freiberg
Akademiestraße 6
09599 Freiberg

Freiberg 2025

Coverbild: Crispin Iven Mokry (CC-BY-NC-SA 4.0)