HELMHOLTZ
CENTRE FOR
ENVIRONMENTAL
RESEARCH – UFZ

GEFTA

26th Kalorimetrietage
June 11 – June 13

ABSTRACT BOOKLET

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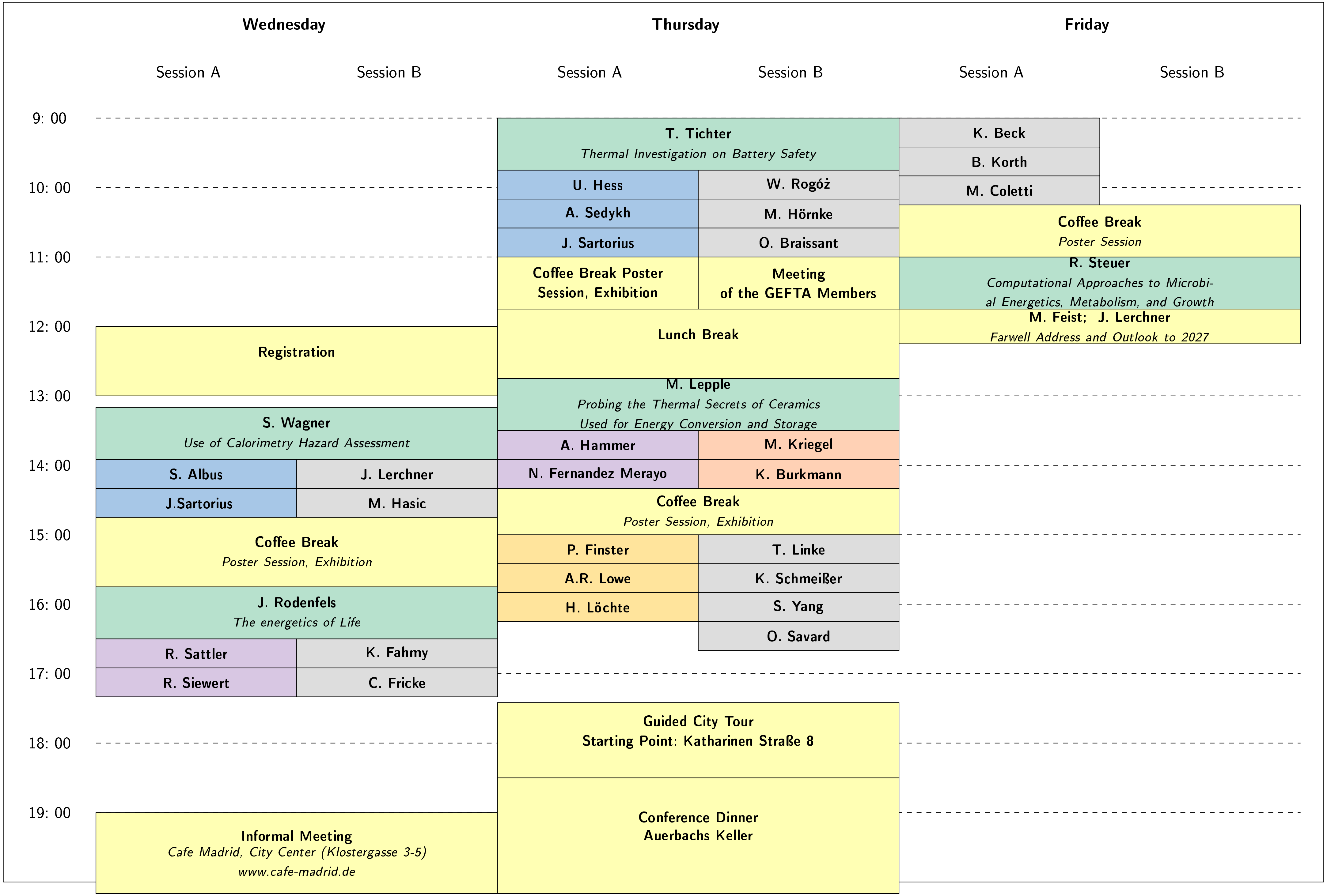

	Wednesday		Thursday		Friday	
	Session A	Session B	Session A	Session B	Session A	Session B
9: 00			**T. Tichter** *Thermal Investigation on Battery Safety*		**K. Beck**	
					B. Korth	
			U. Hess	**W. Rogóż**		
					M. Coletti	
10: 00						
			A. Sedykh	**M. Hörnke**		
					Coffee Break *Poster Session*	
			J. Sartorius	**O. Braissant**		
11: 00			**Coffee Break Poster Session, Exhibition**	**Meeting of the GEFTA Members**	**R. Steuer** *Computational Approaches to Microbial Energetics, Metabolism, and Growth*	
			Lunch Break		**M. Feist; J. Lerchner** *Farwell Address and Outlook to 2027*	
12: 00	**Registration**					
			M. Lepple *Probing the Thermal Secrets of Ceramics Used for Energy Conversion and Storage*			
13: 00						
	S. Wagner *Use of Calorimetry Hazard Assessment*					
			A. Hammer	**M. Kriegel**		
14: 00	**S. Albus**	**J. Lerchner**	**N. Fernandez Merayo**	**K. Burkmann**		
	J.Sartorius	**M. Hasic**	**Coffee Break** *Poster Session, Exhibition*			
	Coffee Break *Poster Session, Exhibition*					
15: 00			**P. Finster**	**T. Linke**		
			A.R. Lowe	**K. Schmeißer**		
	J. Rodenfels *The energetics of Life*					
			H. Löchte	**S. Yang**		
16: 00						
				O. Savard		
	R. Sattler	**K. Fahmy**				
	R. Siewert	**C. Fricke**				
17: 00						
			Guided City Tour **Starting Point: Katharinen Straße 8**			
18: 00						
			Conference Dinner **Auerbachs Keller**			
19: 00	**Informal Meeting** *Cafe Madrid, City Center (Klostergasse 3-5)* *www.cafe-madrid.de*					

Day 1 | Block 1 - Oral Presentations

June 11th, 13:00 PM – 14:45 PM CEST

HALL A: Process Safety (Chair: Steffen Neuenfeld)

Invited Lecture:

ID: 12001
13:10 - 13:55

On the Use of Calorimetry in Chemical Reaction Hazard Assessments

Dr. Sven Wagner[1]

[1] *TÜV SÜD Schweiz, Process Safety Competence Center, Basel, Switzerland*

Calorimetry is an essential tool in the assessment of chemical reaction hazards, offering quantitative insight into thermal behavior and decomposition risks during scale-up and process development. Gathering calorimetric data and extrapolating them to plant scale to define an envelope of safe operation can be done by using a systematic chemical reaction hazard assessment methodology.
This methodology would have allowed to foresee that for the drying of sodium dichloroisoRoyal-Blueurate dihydrate a process change from using an open fluidized bed dryer to a closed double cone dryer can lead to an explosion as occurred at Optima Belle[1]. To study the effects of deviations/changes systematically, guide words similar to the ones in HAZOP studies can be used (e.g. too high temperature, too low temperature, too much addition, less addition etc) and applied to various unit operations.
Finally, if process control still leads to a too high risk of a thermal runaway, risk reducing measures must be implemented. Typically, only a limited number of measures are available to prevent a runaway. Criticality classes in combination with calorimetric data can be used to identify which ones are feasible. However, once measures are deemed appropriate, they need to be designed with due considering of process specifics e.g. mixing times, response times, independence of the measure to the initiating deviation.
Chemical reaction hazard assessments of chemical waste streams are still a challenge particularly due to the variability of composition, the unpredictability of mixed or aged materials and the limitations of existing pragmatic calorimetric methods when applied to waste characterization.

References:

1. U.S. Chemical Safety and Hazard Investigation Board, *Fatal Chemical Decomposition Reaction and Explosion at Optima Belle LLC*, Investigation Report published July 6th, 2023

Decomposition Kinetics of Peroxide Cocktails applying High-Pressure Calorimetry

ID: 10660
13:55 - 14:20

Svenja Albus[1], *Prof. Dr. Markus Busch*[1]

[1] *TU Darmstadt*

Beyond understanding process dynamics, process modelling and digital twins are increasingly important tools. A reliable database at process conditions is essential for a valid modelling approach. Peroxides play a crucial role in high-pressure polymerization processes, initiating the reaction and affecting the temperature profile of the reactor. The right choice of initiator can help to optimize the process. Moreover, peroxides can be combined to cocktails, extending their range of applications and allowing the operator to fine–tune the process. However, there is a significant lack of understanding the peroxide cocktail decomposition kinetics under relevant process conditions.

Buback[1] used optical methods to investigate the decomposition of single peroxides. Transitiometers are used here to determine peroxide cocktail decomposition kinetics, since isobaric conditions up to $2000\,\mathrm{bar}$ can be set. The high heat-flow- in combination with a high-temperature-resolution of the transitiometer (1344 thermocouples, Tian-Calvet design) enables a precise determination of kinetic parameters.

Transitiometry proved to be a good method to study the decomposition of peroxide(cocktails). In addition to high reproducibility of measurements and kinetic parameters, good agreement with literature results was found. Despite overlapping decomposition signals in cocktails, a method was developed to determine the kinetics of peroxide decomposition separately.

Varying type and concentration of peroxides in cocktails and external influences such as pressure, matrix and heating rate, a better understanding of their decomposition kinetics and mutual influence on each other was achieved. The effects of peroxide cocktails on the process and product properties were tested during the LDPE process. With the far-reaching aim of ultimately being able to design peroxide cocktails for specific industrial processes and different polymer properties.

References:

1. M. Buback et al., Z. Phys. Chem., 1999, 210, 199–221

Continuous Heat Accumulation Pressure Vessel Test (Conti-DWS)

ID: 10833
14:20 - 14:45

Dr. Jana Sartorius[1]; Dr. Johannes Schröder[1]; Dr. Markus Gödde[1]

[1]BASF SE, Ludwigshafen am Rhein, Germany

The operation of chemical plants requires a thorough understanding of the safety characteristics associated with chemical processes. Accurate derivation of these characteristics from representative samples is essential, particularly for complex reaction systems sensitive to minor process variations or external influences. Multi-stage heterogeneously catalyzed reactions involving catalyst activation and various transitional states exemplify such systems.

The Continuous Heat Accumulation Pressure Vessel Test (Conti-DWS) is designed to replicate all stages of these reactions, enabling the generation of representative samples in the setup with minimized external impacts. By this, a reliable assessment of the decomposition behavior of complex multi-stage processes by adiabatic calorimetry is enabled. The unique feature of the Conti-DWS, compared to other adiabatic calorimeters, is its adjustable flow configurations, facilitating the dosing of liquids and gases under diverse conditions and allowing for the examination of steady-state operation independent of transient startup phenomena.

The primary objective of the Conti-DWS is to establish a steady-state operation that reflects the initial conditions of a cooling failure scenario. After adjusting this steady-state, the inlet and outlet of the measurement cell are sealed, and the reaction mixture is maintained under adiabatic conditions. This methodology enables the quantification of critical safety-related parameters, including induction time, adiabatic temperature rise, and the gradients of temperature and pressure. Such data are invaluable for safety assessments and kinetic studies.

The flexibility of the Conti-DWS renders it an adaptable instrument for R&D within the chemical industry. Consequently, it enhances methodologies for the investigation and evaluation of continuous reactions in multiphase reactors, thereby contributing significantly to the definition of safe operational windows in production facilities.

Thermogenesis in flight muscles of Drosophila melanogaster – a chip calorimetric study

ID: 10879
13:55 - 14:20

Dr. Johannes Lerchner[1]; Yan A. Reis[2]; Thalita Lúcio[2]; Prof. Marcus F. Oliveira[2]

[1] TU Bergakademie Freiberg, Faculty of Chemistry, Physics and Biosciences, Institute of Physical Chemistry, Freiberg, Germany
[2] Universidade Federal do Rio de Janeiro, Institute of Medical Biochemistry, Rio de Janeiro, Brasil

Mitochondria play a central role in energy metabolism, integrating cellular processes through bidirectional signaling. Mitochondrial redox shuttles regulate the cytosolic and mitochondrial NAD(P) balance and transfer reducing equivalents to mitochondria. The glycerol-phosphate shuttle (GPSh) interconnects glucose and lipid metabolism with oxidative phosphorylation (OXPHOS). While GPSh role in electron transfer is established, its impact on energy efficiency and glycolytic flux remains largely unknown. We hypothesized that GPSh sustains glycolysis by regenerating cytosolic NAD$^+$, but at the cost of lower energy efficiency due to weak coupling between respiration and ATP synthesis, leading to increased heat production.
Using Drosophila melanogaster flight muscle as a model and measuring its heat production by a chip calorimeter, we found that glucose-driven heat production is primarily mediated by OXPHOS, mainly through complex III, as antimycin A inhibited thermogenesis by $\approx 90\%$. The specificity of iGP1 as a true mitochondrial glycerol-3-phosphate dehydrogenase (mGPDH) inhibitor in this model was confirmed via high-resolution respirometry, with an IC50 of $50\,\mu\mathrm{M}$. Strikingly, iGP1 reduced thermogenesis by $\approx 80\%$, underscoring the key role of GPSh in maintaining the NAD$^+$ redox balance for glycolysis. Heat production during ATP synthesis with complex I substrates was comparable to that of G3P oxidation. However, under non-phosphorylating conditions, heat production mediated by complex I substrate oxidation was significantly lower than from mG3PDH, suggesting that GPSh is intrinsically less coupled to ATP synthesis. In summary, GPSh serves as a key mechanism for sustaining NAD$^+$ regeneration in glycolysis but operates with low energy efficiency, leading to increased heat production in highly metabolically active tissues such as insect flight muscle.

Exploring aerobic and anaerobic contributions to thermogenesis in brown adipose tissue

ID: 10875
14:20 - 14:55

Mersiha Hasic[1]

[1]*Technical University of Munich, School of Life Sciences, Chair for Molecular Nutritional Medicine, Munich, Germany*

Brown adipose tissue (BAT) is a specialized fat depot capable of generating heat, helping small mammals defend their body temperature when exposed to cold conditions. This process, known as non-shivering thermogenesis (NST), is catalyzed by uncoupling protein 1 (UCP1) in the inner mitochondrial membrane. UCP1, as the name indicates, uncouples respiration from ATP production, allowing energy from nutrient oxidation to be released as heat rather than stored. Typically, BAT thermogenesis is estimated by measuring oxygen consumption rates (respirometry) and calculating heat output based on assumed caloric equivalents (indirect calorimetry). However, this method captures only oxygen-dependent (aerobic) metabolism and may miss contributions from anaerobic processes.

In our work, we directly compare oxygen-based estimates with direct measurements of heat production in BAT. We used tissue explants of BAT, prepared under conditions optimized for preserving tissue structure, oxygen diffusion, and functional integrity. Basal and noradrenaline-stimulated respiration was measured using a Clark-type oxygen electrode, while total heat release, reflecting both aerobic and anaerobic components, was measured with a chip calorimeter [1].

Our preliminary calorimetry experiments detect approximately 15% more heat production than expected from oxygen consumption alone under basal conditions. This suggests that oxygen-independent pathways may fuel a portion of ATP turnover and thermogenic activity in BAT.

These findings indicate that non-oxidative metabolism could contribute to thermogenesis, possibly by supporting ATP-dependent processes such as futile lipid cycling. Understanding the balance between aerobic and anaerobic contributions is essential for a full picture of energy expenditure in thermogenic tissues.

References:

1. Lerchner J, Hervas LS, Bícego KC et al. (2024) *A device for rapid calorimetric measurements on small biological tissue samples.* J Therm Anal Calorim

Day 1 | Block 2 - Oral Presentations

June 11th, 15:45 PM – 17:20 PM CEST

HALL A: Environmental Science and Macromolecules (Chair: Stefan Sarge)

Invited Lecture:

ID: 11033
15:45 - 16:30

Energetics of Biological Systems

Dr. Jonathan Rodenfels[1]

[1]Max Planck Institute of Molecular Cell Biology and Genetics, Institute of Physical Chemistry, Dresden, Germany

Living biological systems are metabolically active, open systems that constantly exchange matter and energy with their environment. At the core of this lies cellular metabolism, an interconnected network of chemical reactions that transforms environmental nutrients into the mass and free energy that support organismal homeostasis, growth, and development. Because the matter and energy fluxes sustained by metabolism keep cells far from thermodynamic equilibrium, it has long been speculated that energy dissipation poses essential constraints to life. To understand how cells and organisms function, we must determine how metabolic energy is transformed and partitioned among the complex cellular processes necessary for life at any scale, from isolated biochemical networks to quiescent and highly proliferative cells to organismal growth and development. Here, I will discuss our approaches on how we combine experimental calorimetric heat dissipation measurements, perturbations, imaging, and metabolomics with theoretical non-equilibrium thermodynamics approaches to determine the energetics that drive organismal growth and the progression of metazoan embryonic development.

New insights on crystal growth and polymorphic states in long chain polyamide 10.12

ID: 11064
16:30 - 16:55

Rene Sattler[1]; Dr. Heiko Huth[2]; Dr. Varun Danke[3]; Prof. Dr. Mario Beiner[2]

[1] Martin-Luther-University Halle-Wittenberg, Faculty of Natural Sciences II, Halle (Saale), Germany
[2] Fraunhofer-Institute for Microstructure of Materials and Systems IMWS, Halle (Saale), Germany
[3] Evonik Operations GmbH, Research, Development & Innovation, Marl, Germany

In this talk we report about the influence of crystallization kinetics on crystalline states of polyamide 10.12 (PA10.12). Results from Ultra-Fast Scanning-Calorimetry (UFSC) are reported and compared to crystallographic data from Wide-Angle X-ray Diffraction (WAXD). PA10.12 is a polymorphic material that can crystallize in the triclinic α, monoclinic β and hexagonal γ phase. Temperature-dependent WAXD measurements reveal that the α and γ phase constitute an enantiotropic system, i.e. the α phase is the preferred phase at ambient temperatures after slow cooling the melt below the Brill transition temperature T_B of about $90\,^{\circ}\mathrm{C}$. Above T_B a reversible solid-solid phase transition to the γ phase occurs.

Isothermal UFSC measurements are performed after quenching the sample to an amorphous state. For isothermal crystallization temperatures T_c below T_B two distinct melting peaks occur during heating while a single melting peak is found after isothermal crystallization at temperatures above T_B. Two-step isothermal crystallization experiments are performed at selected temperatures that provide further evidence for the growth of different polymorphic states. However, the interpretation of multiple phase transitions observed in UFSC heating scans is extremely complex for polymorphic systems and requires more than calorimetric analysis alone. We compare the isothermal UFSC results with crystallographic WAXD data and scenarios for the growth of different polymorphic states are discussed.

Non-isothermal UFSC measurements with various combinations of cooling and heating rates are performed. We demonstrate that nucleation and crystal growth can be suppressed completely. The critical cooling rate, at which crystallization during cooling is prevented, is about $2.500\,\mathrm{K\,s^{-1}}$. Interestingly, cold crystallization during heating can also be suppressed by suitable combinations of rapid cooling and fast heating. These results are discussed in the light of crystal nucleation and growth.

Utilization of lignin: Thermochemical effects of depolymerization

ID: 10856
16:55 - 17:20

Dr. Riko Siewert[1]; Prof. Dr. Sergey P. Verevkin[2]; Prof. Dr. Karsten Müller[1]

[1]University of Rostock, Institute of Technical Thermodynamics, Rostock, Germany
[2]University of Rostock, Institut für Chemie, Rostock, Germany

Lignin is a complex biopolymer, yet it can be characterized by a limited set of binding motifs. The stability of these bonds plays a critical role in lignin depolymerization. However, to date, only theoretical studies have investigated the homolytic cleavage of these binding motifs. The present work explores the more realistic heterolytic cleavage of these bonds using experimental thermodynamic methods. One of the primary experimental techniques employed is combustion calorimetry, which allows the calculation of standard enthalpies of formation from combustion enthalpies via Hess's law. By utilizing these enthalpies and a progressively more complex series of model compounds, it is possible to estimate the relative stability of different lignin bond types. Additionally, this approach helps elucidate the structural factors responsible for the varying stabilities of model compounds and actual lignin components. A particular focus is placed on hydroxyl groups located in proximity to ether groups. These bonding motifs differ from pure ethers due to the formation of intramolecular hydrogen bonds, which are crucial in reaction thermodynamics, especially when reactants and products possess hydrogen bonds of differing strengths. Depending on the relative stabilization of the reactants and products, a higher molar fraction of the more stabilized species will prevail at equilibrium. For the cleavage of compounds representing lignin bonding motifs, it has been demonstrated that the presence of a hydroxyl group near the ether linkage significantly influences the enthalpy of formation, resulting in a notable shift in reaction enthalpy compared to pure ethers. This observation contributes to the improvement of lignin depolymerization processes in which the cleavage sequence of different binding motifs is thermodynamically determined.

Retrieving pathway-specific substrate utilization rates from microbial heat flow curves

ID: 10675
16:30 - 16:55

Prof. Dr. Karim Fahmy[1]*; Jana Oertel*[1]*; Nataliya Safronova*[2]*; James Sáenz*[2]

[1] *Helmholtz-Zentrum Dresden - Rossendorf, Inst. Resource Ecology, Germany*
[2] *B CUBE - Center for Molecular Bioengineering, Technical University Dresden, Germany*

Isothermal microcalorimetry (IMC) is an extraordinarily sensitive tool for monitoring metabolic activities of microorganisms. It allows determining yields as well as rates of the underlying biochemical reactions. Although technically independent of each other, rates and yields may couple by metabolic regulation. Also experimentally, they are not always easily determined. The amount of metabolized substrate, required for yield estimates, is not always unambiguously obtained from time-integrated IMC curves ("enthalpy domain"). Likewise, a multitude of growth models is used in a rather arbitrary way to model IMC data in the "time domain". These and other factors render comparability of IMC data from different labs difficult.

Using the simplest glycolysis-based anaerobic metabolic network, i.e., that of the genome-minimized bacterium JCVIsyn3.b derived from the pathogenic group of Mycoplasma, we attempted a rigorous calorimetric analysis of metabolic yield and rate parameters. IMC data were modelled by an extended calorimetric Monod equation (ECME) which applies to culture growth rather than substrate-dependent per-cell metabolic activity as originally defined by Monod. We identified pathway-specific heat yields for biomass- and non biomass-related metabolism and show how cell division rate an cell mass couple in response to the plasma membrane lipid composition in this smallest life-supporting system on earth. Using the validated benchmarks of heat flow modelling, we exemplify with IMC data from the fungus *Schizophyllum commune* – in transit from oxidative and fermentative metabolism –, how yield and rate estimates can be obtained systematically using the web-tool METABOLATOR.

Engineering and Evaluation of a Calorespirometer for Real-Time Microbial Activity Monitoring

ID: 10878
16:55 - 17:20

Prof. Dr. Christian Fricke[1,2]*; Eliana Di Lodovico*[2]*; Prof. Dr. Thomas Maskow*[3]*; Prof. Dr. Gabriele Ellen Schaumann*[2]

[1] *Duale Hochschule Sachsen - Staatliche Studienakademie Riesa, Riesa, Germany*
[2] *University of Kaiserslautern-Landau, Department of Natural and Environmental Sciences, Environmental and Soil Chemistry Lab, Landau, Germany*
[3] *Helmholtz-Centre for Environmental Research – UFZ, Leipzig, Germany*

Microbial metabolic activity in both simple (pure cultures) and complex (e.g., soil) systems can be assessed using calorespirometry, which simultaneously measures heat production rate (Rq, in W) and $\mathrm{CO_2}$ production rate (RCO_2, in $\mathrm{mol\,s^{-1}}$). In complex systems like soil, this provides valuable insights into processes such as soil organic matter turnover. Conventional methods often require two separate instruments: an isothermal microcalorimeter for Rq and a respirometer for RCO_2. Alternatively, small ampoule-based calorimetric setups $<(20\,\mathrm{mL})$ trap CO_2 and measure the heat of both metabolism and $\mathrm{CO_2}$ absorption. However, this approach has limitations, including the need for separate experiments and the risk of oxygen depletion, which can alter microbial activity.

To overcome these challenges, we developed a novel calorespirometric system that combines a conventional respirometer (top of the measurement channel), which detects conductivity changes in KOH solution due to $\mathrm{CO_2}$ absorption, with a calorimetric unit (bottom of the channel) containing a heat flow sensor, heat sink, and sample vessel. This design allows for the simultaneous measurement of Rq and RCO_2 in a single experiment—without $\mathrm{CO_2}$ trapping in the calorimetric vessel and with sufficient oxygen supply thanks to a large headspace ($>100\,\mathrm{mL}$).

In order to validate the system, we used yeast growing on glucose as a model. Experimental data aligned well with theoretical values for metabolic heat release and $\mathrm{CO_2}$ production, confirming the accuracy of the setup. A multichannel version was then developed and successfully applied to measure substrate-induced microbial activity in soil, enabling simultaneous Rq and RCO_2 measurements. This demonstrates the system's potential for high-throughput microbial analysis in complex, heterogeneous environments.

Day 2 | Block 1 - Oral Presentations

June 12th, 9:00 AM – 11:00 AM CEST

HALL A: Process Safety (Chair: Markus Gödde)

Invited Lecture:

ID: 12006
09:00 - 09:45

Thermal Investigation on Battery Safety

Dr. Tim Tichter[1]

[1] *Bundesanstalt für Materialforschung und -prüfung (BAM), Safety of Dangerous Goods Packagings and Batteries, Berlin, Germany*

The transportation and storage of lithium-ion batteries (LIB) — damaged or in an undefined state — is a major safety concern for regulatory institutions. Damaged LIBs pose the risk of a so-called thermal runaway (TR), a strongly exothermic reaction with the formation of gases, flames or even an explosion of the battery. The relevance of this issue is underlined by the number of fires that have occurred at recycling centers in the recent past. One solution to circumvent a TR is given by thermal passivation (i.e. deep-freezing) of batteries. Practically, this method is already used and temperatures below $-60\,^\circ\mathrm{C}$ are considered safe.

In this talk, the parameter battery safety is revisited under the premise of heat-transfer and activation energies. At first, mechanically initiated TRs are compared for different cell chemistries, cell sizes, and temperatures, revealing that the threshold of thermal passivation is vastly system specific. Combining these results with differential scanning calorimetry underlines that the hazard potential of a battery is not necessarily eliminated by freezing the electrolyte. Instead, the potential for a TR needs to be regarded as a multivariant function of energy content, cell-voltage, chemical stability, and electrokinetic performance. Since the latter parameter is known to be vastly temperature-dependent, it is addressed in detail by a low-temperature electrokinetic study of different types of LIB. In this context, it is demonstrated that batteries are kinetically active even at temperatures well below the freezing point of the electrolyte and that their instantaneous power output is resembled sufficiently via Arrhenius' law.

To get a detailed understanding of cell-specific heat release during and prior to a TR, data from accelerated rate calorimetry will be discussed for various cell types at different state of charge and state of health. This will eventually provide a conclusive picture how a cell-internal TR-propagation takes place and which parameters need to be deliberately tuned under the premise of battery safety.

Assessing Reactive Hazards: What is the right Tool?

ID: 11065
09:45 - 10:10

Uwe Hess[1]; Sara Roger[2]; Jim Burelbach[2]

[1] ProSense GmbH, Aretinstr. 24, Munich, Germany
[2] Fauske and Associates LLC, Burr Ridge, Illinois, USA

Evaluating reactive chemical hazards is a crucial part of plant safety. Selecting the best experimental approach to address reactive hazards depends on a variety of factors including identifying the objective, details of the reaction, and potential equipment limitations. An overview of various laboratory experimental techniques recommended for developing a safe chemical process will be discussed with focus on evaluating heat and pressure generation through the use of calorimetry. Techniques discussed include Differential Scanning Calorimetry (DSC), Accelerating Rate Calorimetry (ARC), isothermal heat flow calorimetry (TAM, Calvet HT), and low thermal inertia calorimetry (VSP2 & ARSST) with example data of each. The pros and cons of the various techniques, recommendations for collecting quality data, and their typical safety applications such as heat of reaction, adiabatic temperature rise, instantaneous heat flow, adiabatic time to maximum rate (TMR), self-accelerating decomposition temperature (SADT), and emergency relief requirement are discussed with the use of a case study on allyl phenyl ether.

Thermal Properties of LPSCl Solid Electrolytes

ID: 10858
10:10 - 10:35

Dr. Alexander Sedykh[1]; *Michael Grube*[2]; *Prof. Dr. Wolfgang G. Zeier*[3]; *Prof. Dr. Jürgen Janek*[4]; *Prof. Dr. Maren Lepple*[1]

[1] *Justus Liebig University Giessen, Institute of Inorganic and Analytical Chemistry, Giessen, Germany*
[2] *Fraunhofer Institute for Surface Engineering and Thin Films, Braunschweig, Germany*
[3] *University of Münster, Institute of Inorganic and Analytical Chemistry, Münster, Germany*
[4] *Justus Liebig University Giessen, Institute of Physical Chemistry, Giessen, Germany*

Sulfide solid electrolytes exhibit the highest ionic conductivities ($1\text{-}10\,\mathrm{mSv\,cm^{-1}}$) of all solid electrolytes (SE) and are on par with liquid electrolytes.[1] Among SEs, lithium argyrodites $Li_{6-x}PS_{5-x}CL_{1+x}$ are the most promising due to their decent cost efficiency.[1] Understanding these materials' thermal stability is critical for the commercialization of solid-state batteries. However, the reported thermal properties of Li_6PS_5Cl are inconsistent in the literature. Some articles report its stability as high as $900\,^{\circ}\mathrm{C}$,[2] while in other investigations, the thermal decomposition occurs already in the 200-400$^{\circ}\mathrm{C}$ range.[3] Other compositions, such as $Li_{5.5}PS_{4.5}Cl_{1.5}$, are scarcely thermally investigated.

We investigated the thermal stability of Li_6PS_5Cl from various sources using simultaneous thermogravimetry and differential thermal analysis coupled with mass-spectrometry (TG-DTA-MS) and simultaneous thermogravimetry and differential scanning calorimetry (TG-DSC). As found out in this work, the thermal stability of $Li_{6-x}PS_{5-x}CL_{1+x}$ significantly depends on the synthesis method and manufacturer.

We propose a straightforward method to evaluate sulfidic SEs purity and stability: to analyze the sample by TG-DSC in an atmosphere switching from inert to oxidative at an elevated temperature. This prevents instrument damage risks from potential corrosive material spilling and also provides the behavior of the sample in different atmospheres, inert and oxidative, in a single experiment.

Additionally, experimental thermodynamical data of specific heat capacities and enthalpies of combustion, and therefore enthalpy of formation, are collected for both, Li_6PS_5Cl and $Li_{5.5}PS_{4.5}Cl_{1.5}$. This allows the thermal modelling of solid-state batteries and strategic planning for their recycling.

References:

1. T. Schmaltz et al., Adv. Energy Mater. 2023, 13, 2301886.
2. S. Wang et al., InfoMat 2022, 4, 1-16.
3. R. F. Indrawan et al., Chem. Mater. 2023, 35, 2549-2558.

Determination of the Self-Accelerating Decomposition Temperature (SADT) of Auto-Catalytic Substances

ID: 10849
10:35 - 11:00

Dr. Julian Sartorius[1]; Dr. David Zink[1]; Dirk Bender[1]; Sebastian Kimpel[1]

[1] consilab Gesellschaft für Anlagensicherheit mbH, Frankfurt/ Main , Germany

The surrounding temperature where the heat loss of a container equals the heat release rate of the substance is called SADT. The SADT is an important criterion for the safety evaluation of storage and transport of chemicals and is determined via calorimetry, detailed in the UN Manual of Tests and Criteria, Revision 8 (2023) in the H-test series. These tests are well established and yield good results for most substances. This is, however, not the case for auto-catalytic substances.

The thermal stability of auto-catalytic substances is not only dependent on the testing/process temperature, but additionally heavily dependent on its thermal history. These substances show an increasing heat generation under isothermal conditions which leads to a maximum before decreasing due to conversion. These properties complicate the safety-related evaluation of auto-catalytic substances, because the typical methods and criteria do not apply anymore.

Little guidance is found in the guidelines and regulations concerning the determination of the SADT of auto-catalytic substances. Solely for the UN test H.3 in isothermal micro-calorimeters it is noted that the test may take auto-catalytic effects into account, when measuring times are long enough (e.g. > 100 hours).

The results of that method are based on the maximum heat generation observed at the respective temperature and very conservative from a safety-related viewpoint. This method is often too conservative for auto-catalytic substances and results in unfeasibly low SADTs. In this work we propose a new method to determine the SADT of auto-catalytic substances. First an adiabatic pressure/heat accumulation test based on UN test H.2 is performed. The kinetics are evaluated at the auto-catalytic saturation (maximum auto-catalysis). Based on the kinetics the SADT is determined. The results are validated in a Tian-Calvet- and a micro-calorimeter.

The proposed method allows to determine a feasible SADT meeting safety-related standards.

Calorimetric and spectroscopic analysis of methylation influence on ligand-protein interaction

ID: 10661
09:45 - 10:10

PhD Wojciech Rogóż[1]*; MSc Aleksandra Owczarzy*[1]*; MSc Karolina Kulig*[1]*; PhD, DSc Małgorzata Maciążek-Jurczyk*[1]

[1]*Faculty of Pharmaceutical Sciences in Sosnowiec, Medical University of Silesia, Poland*

Pharmacokinetics of chemicals can be changed by modifications of the compounds' functional groups. The most important protein involved in the transport of drugs in the blood is human serum albumin (HSA). The interactions between HSA and ligands usually lead to the modifications in proteins' conformation, at the level of proteins' secondary and tertiary structures.
The aim of the study was to characterize the interactions between HSA and ligands: gallic (GA), syringic (SYR) and eudesmic (EUD) acids. All samples were prepared in phosphate buffer ($0.05\,\mathrm{mM}$; pH 7.4) and analyzed by calorimetric (nanoITC, TA Instruments) and spectropolarimetric (JASCO International Co., Ltd.) techniques. The concentrations of HSA were 1×10^{-4} $\mathrm{mol\,dm^{-3}}$ (nanoITC), 3×10^{-6} $\mathrm{mol\,dm^{-3}}$ (far-UV CD) and 2×10^{-5} $\mathrm{mol\,dm^{-3}}$ (near-UV CD), while concentrations of ligands stock solution were 1.17×10^{-3} $\mathrm{mol\,dm^{-3}}$ (nanoITC), 3×10^{-5} $\mathrm{mol\,dm^{-3}}$ (far-UV CD) and 2×10^{-4} $\mathrm{mol\,dm^{-3}}$ (near-UV CD).
The values of the association constants for the HSA binding reaction with GA, SYR and EUD were $4.11(\pm 0.90) \times 10^5$ $\mathrm{dm^3\,mol^{-1}}$, $6.44(\pm 1.31) \times 10^4$ $\mathrm{dm^3\,mol^{-1}}$ and $2.01(\pm 0.09) \times 10^5$ $\mathrm{dm^3\,mol^{-1}}$, respectively. The HSA affinity towards ligands was moderate. All processes of (HSA-ligand)complex formation were spontaneous ($\Delta G < 0$) and exothermic ($\Delta H < 0$). Both (HSA-GA)complex and (HSA-SYR)complex were stabilized by ionic and hydrophobic bonds while hydrogen bonds and van der Waals interaction probably played a key role in (HSA-EUD)complex stability. All ligands induced conformational changes of HSA at the tertiary structure level in the regions rich in Phe, Tyr and Trp residues. At the same time, the binding of SYR and EUD to HSA resulted in a decrease in the percentage of a-helix structure.
It can be concluded that methylation of the ligand's hydroxyl groups affects its binding to HSA.

This research was funded by Grant *BNW-1-009/K/4/F, BNW-2-049/K/4/F, BNW-2-048/K/4/F, BNW-2-110/K/4/F* from the Medical University of Silesia, Poland.

Lipid Phase Transitions in Membrane Biophysics

ID: 12002
10:10 - 10:35

Dr. Maria Hoernke[1,2]*; Bjarne Bräuer*[1]*; Mehriddin Yodgorov*[1]*; Shuai Shi*[2]*; Katharina Beck*[2,3,4]

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[3]*University of Augsburg, Physiology, Institute of Theoretical Medicine, Augsburg, Germany*
[4]*University of Augsburg, Physiology, Experimental Physics I, Institute of Physics, Augsburg, Germany*

In membrane biophysics, lipid phase transitions in model membranes can be used to indirectly report about induced membrane perturbations, both in the chain region (first example) or driven by the lipid head groups (second example).
(1) Archaeal lipids differ from typical bacterial or eukaryotic phosphoester lipids by their ether-linkage, a different stereochemistry, but also by their isoprenoid chains instead of linear alkyl chains. These lipids are designed to maintain membrane function also under harsh pH, temperature or slat conditions that archaea evolved to live at. Therefore, archaeal lipids are discussed for potential delivery of vulnerable drugs via the oral path. We investigated the behavior of mixed membranes composed of die-ether lipids and classical phosphoester lipids by several methods that are sensitive to the lipid phase state or reporting about phase transitions, such as differential scanning calorimetry, attenuated total reflection FT-IR, and laurdan fluorescence. The membrane behavior is dominated by small amounts of branched lipids and results and advantages of the various methods can be compared.
(2) Antimicrobial peptides or polymers are supposed to act on the integrity of the bacterial cytoplasmic membrane. Many mechanistic studies use model membranes to assess various types of perturbations. With a combination of methods including differential scanning calorimetry to show lipid demixing, fluorescence spectroscopy to assess membrane fusion, and fluorescence lifetime to characterize membrane leakage, we show how the different effects are connected. Furthermore, the most common model membrane containing PG and PE lipids is found to be biased towards effects that are not relevant in bacteria and modified model membranes are proposed.

Performances of antimicrobial material and antimicrobial coatings assessment using isothermal calorimetry.

ID: 10853
10:35 - 11:00

Dr. Olivier Braissant[1]; Dr. Monika Astašov-Frauenhoffer[2]; Prof. Dr. Gernot Boncat MD[3]

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[2]Universitäres Zentrum für Zahnmedizin Basel (UZB), Basel, Switzerland
[3]Alta Uro AG, Basel, Switzerland

Contrary to many other methods commonly used in biology and microbiology, isothermal microcalorimetry is not limited by the physical nature of the sample. Indeed, it can accommodate liquid samples, but also gel, solid, porous and opaque materials. As a result, it is possible to take advantage of this versatility to test the antimicrobial activity of various surfaces and material. Here, we present a technique using solid agar and materials coated or loaded with antimicrobials. The use of agar media avoids the growth of planktonic cells and promote the bacterial growth as biofilm, in between the surface and the medium. Using such approach we tested several antimicrobial materials and coating over the last years. Metallic implant material coated with silver dope hydroxyapatite or calcium hydroxide showed good efficacy despite the poor solubility and diffusion of both silver and hydroxide. In addition for those implants, calorimetry allowed to use the final implant geometry (a screw) for the testing before animal studies. Similarly, cellulose based dental aligners loaded with antimicrobial essential oils such as cinnamaldehyde and limonene also showed good efficacy. For such aligners the release of essential oils needs to be compensated with intermittent reload of the aligner. However this is still compatible with the use case as aligner have to be removed by patient during meals. Overall, isothermal microcalorimetry proves to be an efficient technique for testing antimicrobial and antibiofilms properties of surfaces and materials. We hope to continue developing such approaches as they contribute to safer implants.

Day 2 | Block 2 - Oral Presentations

June 12th, 13:00 PM – 14:35 PM CEST

HALL A: Environmental Science and Macromolecules (Chair: Dirk Walther)

Invited Lecture:

ID: 12003
12:45 - 13:30

Probing the Thermal Secrets of Ceramics Used for Energy Conversion and Storage

Prof. Dr.-Ing. Maren Lepple[1]

[1] *Justus Liebig University Giessen, Institute of Inorganic and Analytical Chemistry, Giessen, Germany*

Material innovations are often the key to enabling new technologies or making existing processes more efficient. This is particularly important in view of the climate crisis. Ceramic materials play an important role, as they are used in many applications thanks to their versatile outstanding properties, whether as thermal insulation and protective coatings in corrosive atmospheres at high temperatures in gas turbines, as electrode materials and solid electrolytes in batteries, fuel cells and in sensors, as catalyst materials, or as thermoelectrics. Knowledge of the energetics, phase stabilities and phase relations of materials systems of interest enables the reliable use of the new ceramics in technologically demanding applications. Furthermore, thermochemical parameters are important input parameters for thermodynamic modeling of materials systems using the CALPHAD approach, enabling accelerated material development.

For high-temperature applications, such as in gas turbines, knowledge of thermodynamics is of particular importance, as kinetics no longer has a slowing effect on the setting of thermodynamic equilibrium. Here, ceramics are applied to the metallic substrate materials as a protective thermal barrier coating (TBC). Zirconia stabilized with $\sim 7wt.\%$ $\mathrm{Y_2O_3}$ (7YSZ) is the state-of-the-art material due to its good mechanical properties and thermocyclic behavior, low thermal conductivity, high thermal expansion coefficient and high strain tolerance. However, it is only applicable up to $1200\,^{\circ}\mathrm{C}$, due to a phase separation of the metastable phase.[1] Therefore, new materials showing long-term thermal stability must be found to reduce fuel consumption and greenhouse gas emissions. However, the increased temperatures cause experimental difficulties when determining thermodynamic quantities, as the maximum temperatures of the devices used are exceeded. [2] The strategies of material development and the determination of thermochemical and thermophysical properties for different material systems will be discussed.

References:

1. J. A. Krogstad, M. Lepple, Y. Gao, D. M. Lipkin, C. G. Levi, *Effect of yttria content on the zirconia unit cell parameters*, J. Am. Ceram. Soc. 94 (2011) 4548-4555
2. M. Lepple, S. V. Ushakov, K. Lilova, C. A. Macauley, A. N. Fernandez, C. G. Levi, A. Navrotsky, *Thermochemistry and phase stability of the polymorphs of yttrium tantalate, YTaO4*, J. Europ. Ceram. Soc. 41 (2021) 1629-1638

Thermal Analysis Techniques for the Recycling of Polymers

ID: 10678
13:30 - 13:55

Dr. Angela Hammer[1]; Dr. Jürgen Schawe[2]

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The increased demand for plastic products and packaging has led to a rapid increase in the production of polymers. This, in turn, has resulted in an increase in plastic waste. The desire to reduce the waste has created a need to recycle used polymers and return them to the economy as raw material.
To achieve this goal, research and industry need to identify and characterize the polymers involved, as well as develop suitable recycling processes.
Thermal analysis techniques are an ideal way to help accomplish this goal.
The majority of polymers currently produced are made from crude oil, and result in more than 300 million tons of plastic waste per year, most of which is not biodegradable.
The options for dealing with plastic waste are:

- landfill,
- incineration for energy recovery, or
- recycling the material in order to manufacture new polymer materials.

3 different ways of recycling are possible:
Mechanical recycling, chemical or energy recovery by incineration.
Examples for mechanical and chemical recycling will be demonstrated [1].

References:

1. METTLER Toledo UserCom 15, 15, *Quantitative analysis of polyolefine blends*

Isothermal Titration Calorimetry as a Tool for Monitoring Enzymatic Depolymerization of Polyethylene Terephthalate

ID: 11026
13:55 - 14:20

Noelia Fernandez Merayo[1]*; Prof. Dr. Thomas Maskow*[1]

[1]*Helmholtz - Centre for Environmental Research - UFZ, Department of Microbial Biotechnology, Leipzig, Germany*

Plastic production reached 413.8 million metric tons in 2023 with only 9% of plastic waste being recycled globally [1]. As a result, a significant fraction of plastic enters the environment, where it fragments into micro- ($<5\,\mathrm{mm}$) and nanoplastics (NP, $<100\,\mathrm{nm}$). NP's pose a serious threat due to their ability to permeate human tissues. However, plastic waste also represents an untapped source of materials and energy. To harness this potential biotechnologically, efficient enzymes or microbial strains are needed, along with innovative methods for process monitoring and control. Calorimetry is a promising approach, as the heat of reaction reflects conversion in real time and provides thermodynamic variables for predictive models, serving as a process indicator. We investigated the degradation of polyethylene terephthalate (PET), a widely used material in packaging and disposable items.

It has been reported that PET-NP can be enzymatically degraded into oligomers or monomers, such as MHET (2-hydroxyethyl terephthalic acid), terephthalic acid and ethylene glycol [2]. Isothermal titration calorimetry combined with thermokinetic modelling, has be proven capable of determining kinetic, thermodynamic and stoichiometric parameters in a single experiment. The new method was tested using a plant-metagenome-derived cutinase, the LCCICCG. To obtain thermodynamic data and to exclude interference from surface adsorption, we analyzed the hydrolysis of MHET. Complete conversion was observed with an average ester bond cleavage enthalpy of $-54\,\mathrm{kJ\,mol^{-1}}$ for MHET, depending on temperature and pH, confirming a previously quantified value for PET. The results were validated using conventional Ultra Performance Liquid Chromatography.

These findings pave the way for scaling up calorimetric processes, enabling the technical implementation of calorimetry-based process control. Furthermore, the methods and models developed in this study will be tested for their applicability on polymers.

References:

1. Plastics Europe. "*Plastics – the fast Facts 2024*". (2024)
2. Tournier , V., et al., *An engineered PET depolymerase to break down and recycle plastic bottles.* Nature. 580 (7802): p. 216-219. (2020)

Heat capacities of several ordered intermetallic phases in the system Al–Fe–Mn–Ni–Ti

ID: 10989
13:30 - 13:55

Dr. Mario J. Kriegel[1]*; Dr. Alexander Walnsch*[2]*; Prof. Dr. Andreas Leineweber*[1]

[1] *TU Bergakademie Freiberg, Institute of Materials Science, Freiberg, Germany*
[2] *GTT-Technologies, Herzogenrath, Germany*

Thermodynamic data, such as the isobaric heat capacity (c_p), is essential for establishing reliable thermodynamic databases, which serve as the foundation for computer-based materials development methods. Moreover, it is crucial for high-temperature applications where heat transfer plays a significant role, as it heavily affects thermal conductivity. The development of CalPhaD (Calculation of Phase Diagrams) databases, which can describe thermodynamic functions of bulk phases down to $0\,\mathrm{K}$ in a physically meaningful manner, also known as "3rd generation CalPhaD databases", is becoming increasingly important. The thermodynamic functions of phases in higher-order systems are typically described by the Neumann-Kopp rule, which relates the Gibbs energy of an intermediate phase to the individual pure end-member elements. However, this approach often overestimates the heat capacity of the intermetallic compound. Therefore, experimental data is necessary to compensate for these differences and enable the modeling of realistic material behavior.
Intermetallic materials have attracted the attention of scientists for more than one decade because their fields of application range from, e.g., high-temperature structural materials, shape-memory alloys, permanent magnets and hydrogen-storage materials. The focus is placed on intermetallic phases, which are ordered superstructures derived from disordered FCC (*A1*), BCC (*A2*) and HCP (*A3*) solid solutions. Using the classical three-step continuous method, different DSC devices were used in the temperature range from $110\,\mathrm{K}$ bis $870\,\mathrm{K}$ to measure heat capacities experimentally. The c_p values were used, together with c_p data from literature, to describe the temperature dependent heat capacities of the respective phases using an Extended-Einstein model (EE-model). This model is currently widely adopted in the development of multicomponent thermodynamic databases using the CalPhaD approach for a computer-based materials design.

Thermochemistry of RE7P3O18 Rare Earth Oxyphosphates

ID: 11062
13:55 - 14:20

Dr. Konrad Burkmann[1]; Prof. Sergey Ushakov[1]; Ligen Wang[1]; Prof. Qijun Hong[2]; Prof. Alexandra Navrotsky[1]; Prof. Elizabeth Opila[3]; Prof. Dr. Robert Glaum[4]

[1]Arizona State University, School of Molecular Sciences, Tempe, United States of America
[2]Arizona State University, School for Engineering of Matter, Transport and Energy , Tempe, United States of America
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[4]Rheinische Friedrich-Wilhelms-Universität Bonn, Department of Chemistry, Bonn, Germany

Rare earth (RE) oxyphosphates (REOPs) were discovered half a century ago by melting RE orthophosphates in a solar furnace. They composition can be expressed as $(\mathrm{RE_2O_3})_x\,(\mathrm{REPO_4})$ with several stoichiometries reported for each RE (Fig. 1). Their high melting temperatures, structural diversity and high rare earth content are promising for their use as catalysts, thermal and environmental barrier coatings, high temperature ceramics and novel magnetic materials. However, the development of REOPs-based functional materials is hampered by the current paucity of structural and thermodynamic data. Preliminary structure models for several REOPs were suggested but only $\mathrm{Nd_3PO_7}$ and $\mathrm{Eu_3PO_7}$ structures were solved from single crystal diffraction.

This talk will focus on computational and experimental investigation of 7:3 family of REOPs ($\mathrm{RE_7P_3O_{18}}$ RE = La-Tb). The previously suggested structure model was further improved and optimized using ab initio methods and also derived by relaxation of previously reported $\mathrm{La_7V_3O_{18}}$ structure. The several $\mathrm{RE_7P_3O_{18}}$ compounds (Fig. 1) were synthesized by reaction of rare earth oxides and ammonium phosphate and characterized by X-ray diffraction, differential scanning calorimetry and infra-red spectroscopy. The first results of high temperature oxide melt solution calorimetry experiments for determination of enthalpies of formation and heat capacity measurements will be reported. The goal is to benchmark computational results to be used for CalPhaD modeling of $\mathrm{RE_2O_3} - \mathrm{P_2O_5}$. systems.

Day 2 | Block 3 - Oral Presentations

June 12th, 15:15 PM – 16:55 PM CEST

HALL A: Efficiency in Energy Transformations (Chair: Florian Mertens)

Determination of thermophysical properties of battery electrolytes and their components using DSC

ID: 11061
15:00 - 15:25

Philipp Finster[1]; Judith Jung[1]; Prof. Dr. Hans J. Seifert[1]; Dr. Carlos Ziebert[1]

[1]Karlsruhe Institute of Technology (KIT), Institute for Applied Materials - Applied Materials Physics, Department Composites and Thin Films, Eggenstein-Leopoldshafen, Germany

Carbonate-based battery electrolytes are used in most of the commercially available batteries. Due to the increasing need for battery recycling and the demand for higher charging and discharging rates, accurate heat capacity data at elevated temperatures has become essential. However, measuring the thermal properties of battery electrolytes presents challenges like evaporation of the electrolyte within crucibles or potential decomposition due to contact with oxygen or moisture.

In this work we investigated the thermophysical properties of two carbonate solvents: ethylene carbonate (EC) and ethyl methyl carbonate (EMC) using heat-flux Differential Scanning Calorimetry (DSC). We investigated the melting points, melting enthalpies, boiling points and the heat capacity of EC in the temperature range from $263\,\mathrm{K}$ bis $500\,\mathrm{K}$ in heating mode and $493\,\mathrm{K}$ bis $273\,\mathrm{K}$ in cooling mode. The influence of undercooled liquid in EC is also discussed. The heat capacity of EMC was measured between $211\,\mathrm{K}$ bis $360\,\mathrm{K}$ in heating mode. We provide best practice recommendations for sample preparation, calibration, influence of undercooled liquids, influence of evaporation inside a closed crucible and how to measure the boiling point of carbonates using DSC.[1]

Finally, we present an outlook on our ongoing work about changes in melting behavior of electrolytes containing lithium hexafluorophosphate ($\mathrm{LiPF_6}$). The aim is to establish a nondestructive, qualitative approach for probing electrolyte evolution during operation of the battery cells.

High Pressure Scanning Calorimetry to Investigate the Thermal Effects of Liquid Intrusion/Extrusion from Hydrophobic Porous Materials

ID: 10679
15:25 - 15:50

Dr. Alexander Rowland Lowe[1]; Dr. Weiwei Zhao[2]; Prof. Dr. Mirosław Chorążewski[1]

[1]University of Silesia, Faculty of Science and Technology, Katowice, Poland
[2]University of Birmingham, Engineering and Physical Sciences, Birmingham, England

The heat evolved from the process of driving liquid water into and out of a porous hydrophobic matrix is a difficult process that requires advanced differential scanning calorimetric equipment that can accurately control the rate of pressurization with the associated components necessary to resist pressures beyond the liquid intrusion pressure to create a stable calorimetric baseline. This talk will present the scanning transitiometry technique which is used to determine the liquid heat of water intruding into and from ZIF-8. As part of this presentation the experimental technique and the challenges around the experimental design will be presented with experimental data demonstrating that the intrusion process is exothermic and extrusion process is endothermic at $25\,^{\circ}\mathrm{C}$. As well we show that using this technique the heat of intrusion can be manipulated by change the parameters of temperatures, aqueous environment, and crystal size can be adjusted to not only effect the magnitude of the heat of intrusion value but also change the thermodynamic sign. Manipulation of these parameters provide the tools for designing thermal energy storage, energy recover or energy dissipation system which rely on mechanical work to operate.

Funding: This project leading to this application has received funding from the European Union's Horizon 2020 research and innovation programme under Grant Agreement No. 101017858

Investigation of the temperature dependence of molecule accumulation on porous solids using adsorption calorimetry

ID: 12004
15:50 - 16:15

Hendrik Löchte[1]; Christian Bläker[1]; Christoph Pasel[1]; Dieter Bathen[1,2]

[1] *University of Duisburg-Essen, Chair of Thermal Process Engineering, Duisburg, Germany*
[2] *Institute of Environment & Energy, Technology & Analytics (IUTA) e.V., Duisburg, Germany*

The topic of energy storage is becoming increasingly important, particularly as the proportion of renewable energy sources in the electricity mix rises. This is necessary in order to meet peak loads, ensure grid stability and enable flexible and demand-oriented use. In this context, the storage of hydrogen or methane by adsorption on porous metal hydrides or the use of adsorption heat pumps for heat storage are promising technologies.

The heat release as a consequence of adsorption (heat of adsorption) is a crucial design parameter, as both the adsorption capacity and the process kinetics are considerably influenced by temperature.

The enthalpy of adsorption, as a variable of state, can be determined from the heat of adsorption, which is a process variable, by subtracting an RT-term (R: universal gas constant, T: temperature). The adsorption enthalpy provides a measure of the strength of the intermolecular interactions that occur and thus enables conclusions regarding the prevailing adsorption mechanisms.

Adsorption calorimetry is used in this study to investigate the adsorption of molecules on porous solids. The detection of the time-dependent pressure change, which occurs in a defined sensor gas volume as a result of the heat release, enables the experimental determination of the heat of adsorption. The coupling of a volumetric adsorption measuring device with the calorimetric measuring system enables the simultaneous measurement of adsorption isotherms and heats of adsorption as a function of temperature. This consistent measurement data allows the formulation of conclusions concerning the load- and temperature-dependent adsorption mechanisms. On the basis of the data obtained, adsorbents can be specifically optimized for utilization in energy and heat storage processes.

In the oral presentation, the experimental setup, as well as selected results of the temperature dependence of the adsorption enthalpy will be presented and discussed.

Photo-calorespirometry (Photo-CR): A novel method to directly quantify energy conversion mechanisms in light-induced bio-/chemical reactions

ID: 10990
15:00 - 15:25

Tilman Linke[1]*; Prof. Dr. Andreas Schmid*[1]*; Prof. Dr. Thomas Maskow*[2]

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[2]*Helmholtz - Centre for Environmental Research - UFZ, Department of Microbial Biotechnology, Herzogenrath, Germany*

Photo-calorespirometry (Photo-CR) is an innovative method that combines calorimetry (heat production) and respirometry (oxygen turnover) to study photosynthetic processes. A prototype Photo-Calorespirometer was developed by modifying a conventional microcalorimeter with oxygen optodes and a programmable light source. This setup enables real-time monitoring of heat and gas exchange, linking mass and energy balances for dynamic thermodynamic assessment of aquatic phototrophic microorganisms. Applying thermodynamics to photosynthesis, Photo-CR allows for evaluating metabolic feasibility, estimating biosynthetic yields, and quantifying turnover rates. Oxygen-based data offer insights into side reactions like the Mehler reaction or respiration. The method was validated with two model organisms—*Chlamydomonas reinhardtii* (a green alga) and *Synechocystis sp. PCC 6803* (a cyanobacterium) — revealing a strong correlation between calorimetric and respirometric signals, with oxycaloric equivalents ranging from 437–488 $\mathrm{kJ\,mol^{-1}}$. Photo-CR enables real-time measurement of photosynthetic efficiency under different light conditions, making it ideal for dynamic experiments. It can identify optimal lighting regimes, compare strains or mutants, and enhance photobiological productivity. Beyond microalgae, Photo-CR is suitable for studying light-driven reactions in pharmacology and environmental chemistry, including photodynamic drug activation, microplastic degradation, and light-triggered chemical transformations. As an example, we demonstrate its application in the photocatalytic activity of porphyrins (e.g., TMPyP) and the singlet oxygen-mediated transformation of ABDA (9,10-Anthracedenediyl-bis(methylene)dimalonicacid).

Quantifying the energetics of building and maintaining an organism

ID: 11032
15:25 - 15:50

Dr. Kathrin Schmeisser[1]; Dr. Jonathan Rodenfels[1]

[1] Max Planck Institute of Molecular Cell Biology and Genetics, Institute of Physical Chemistry, Dresden, Germany

All organisms are open systems at a non-equilibrium state with their environment; they constantly exchange energy and matter. Their metabolism uses nutrients from the environment and extracts and transforms energy and matter to maintain and build biomass. Thereby they dissipate heat and metabolic waste products, satisfying the 2. law of thermodynamics. Energy dissipation determines the energetic costs and efficiency of energy transduction in an organism. We are interested in describing metabolism in such a quantitative way: How much energy and matter are consumed, conserved and dissipated? What are the energetic physical constraints imposed on living systems? And what are the energetic costs of maintaining a steady state?

We use *C. elegans* quiescent and developing larvae to measure energy and matter exchange with their environment. For this, we combine isothermal calorimetric heat dissipation measurements (aka metabolic rate) with oxygen and food consumption, and metabolic waste excretion. Relating these measurements with morphometrics such as volume and entropy production calculations, we aim to quantify the overall energetics of maintaining and developing an organism. We further can use these data to identify metabolic types describing the biochemical pathways being employed at any given developmental stage. As we measure metabolic rate in a nanowatt resolution, we are also able to identify and quantify the energetic costs of distinct biological processes and aim to establish metabolic signatures of development that could predict potential metabolic outcomes later in live.

Our work for the first time quantifies metabolism in a multicellular species over its whole reproductive cycle and offers non-precedented insights into the energy metabolism of a living organism. It can help to uncover how the transformation and usage of energy sets fundamental constraints on development and life expectancy, which is likely to be conserved across other multicellular species.

Integrated CO_2 Sensing in Isothermal Microcalorimetry for Microbial Heat and Mineralization Measurements in Soil

ID: 10876
15:50 - 16:15

Shiyue Yang[1]; Sven Paufler[1]; Dr. Anja Miltner[1]; Prof. Dr. Matthias Kästner[1]; Prof. Dr. Thomas Maskow[1]

[1]Helmholtz-Centre for Environmental Research – UFZ, Leipzig, Germany

Soil represents the largest reservoir of organic matter in terrestrial systems. Microbial activity is governed by carbon and energy availability. Energy generated by catabolism and carbon input fuel anabolism for biomass synthesis and energy storage. The ratio between heat and CO_2, known as the calorespirometric ratio, is an important indicators of carbon use efficiency and metabolic pathways.

Traditionally, respiration and heat production are measured separately for soil samples, which can result in mismatched data due to soil heterogeneities and differing temporal resolutions. CO_2 fluxes are often quantified via gas chromatography or absorption in alkaline solutions followed by titration or inorganic C analysis. However, the diffusion and absorption time from soil into alkaline solution may result delays in CO_2 measurements and reduce CO_2 partial pressure, interfering with the metabolism of the microbial community. Meanwhile, isothermal microcalorimeters provide continuous heat production rate data but are rarely integrated with online CO_2 measurement, limiting the ability to link energy and mass fluxes in soil systems.

To overcome these limitations, we present an integrated approach using an IMC equipped with a non-invasive infrared CO_2 sensor, enabling simultaneous and continuous measurement of heat and CO_2 production from the same soil sample. The CO_2 sensor is sealed on the lid of a calorimetric ampoule and the heat production is monitored by a Peltier element. For our incubation setup, the soil samples were amended with glucose and incubated at 16% water content and $20\,^{\circ}\mathrm{C}$. This setup enabled continuous monitoring of the CR ratio through the incubation.

With parallel O_2 measurement, additional parameters such as ratio of heat to O_2 consumption and respiratory quotient can be calculated for the entire metabolic process. This methodological advancement enhances the ability to assess mass and energy flows in soil metabolism under various environmental conditions.

What can images bring to thermal analysis?

ID: 11059
16:15 - 16:40

Olivier Savard[1]

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Thermal analysis techniques like DSC, STA, DMA, and TMA have long been used to study material properties, but understanding the exact changes in samples during experiments could be challenging. Visual observation within the furnace of a thermal analysis instrument provides valuable insights into sample positioning, size, shape, and colour changes.

Observing samples during thermal analysis helps in understanding and explaining results. For example, a TGA curve artifact caused by air trapped in a sample could easily be explained if the image of an air bubble burst out of the sample during a measurement.

Visual images can confirm changes in crystalline forms during thermal analysis. For instance, DSC results of Carbamazepine Form I show its melt, recrystallization to Form III, and subsequent melt, with visible images confirming these changes.

Some materials undergo colour changes over specific temperature ranges. Collecting visible images during thermal analysis allows accurate temperature control and study of thermal behaviour and colour changes. Colour analysis using pixel colour information and models like RGB, Lab, and CMYK can quantify these changes.

Microscope-DSCs enable the analysis of small features such as contamination within a polymer matrix or individual layers within a multilayer sample, which standard DSC cannot detect. These systems allow thermal event measurements of features smaller than $10\,\mu m$ with precise temperature control. For example, polymer laminates analysed by microscope-DSC show melting temperatures of individual layers closely matching the raw materials used.

The presentation will cover the advantages of visual observation in thermal analysis techniques (DSC, STA, DMA, and TMA) with real examples demonstrating the power of these techniques. It will also discuss the additional information that can be extracted from visible images, such as RGB values.

Day 3 | Block 1 - Oral Presentations

June 12th, 9:00 AM – 10:15 AM CEST

HALL A: Biophysical Chemistry (Chair: Heike Bunjes)

Temperature-Dependent Lipid Order in Lipid Nanoparticles: Insights from Fluorescence Spectroscopy

ID: 11063
09:00 - 09:25

Katharina Beck[1]; Anna Nolde[1]; Dr. Nicolas Färber[1]

[1]University of Augsburg, Institute for Theoretical Medicine, Augsburg, Germany

Lipid nanoparticles (LNPs) represent a promising avenue of research in the field of drug delivery systems, with particular relevance to the development of RNA-based vaccines and therapeutics. However, a deeper understanding of the formulation concepts behind LNPs is essential for their focused optimization and overcoming obstacles such as storage instability. We aim to make a substantial contribution to this field of study by directing our research towards a detailed examination of the lipids.

The use of solvatochromic dyes, such as Laurdan, enables the precise measurement of lipid order. Laurdan is a unique probe that integrates into membranes and lipid systems, where its fluorescence properties are highly sensitive to the polarity of the surrounding environment. This allows for the examination of packing density and lipid order. By employing fluorescence spectroscopic measurements with the Lipid State Observer (LISO), we quantify the lipid order through the calculation of the generalised polarisation (GP) based on fluorescence emission spectra [1].

Notably, this approach allows us, for the first time, to analyse the lipid order of LNP-formulations like the COVID-19 vaccine at sub-zero temperatures in the frozen state. The phase transition temperatures of LNP formulations can further be estimated by measuring GP as a function of temperature, providing an additional valuable characterisation of these systems. At present, we are engaged in an investigation into the potential correlations between the lipid order and other critical properties of LNP, including encapsulation efficiency, transfection efficiency, and storage stability.

References:

1. Färber, Nicolas and Westerhausen, Christoph. *"Broad lipid phase transitions in mammalian cell membranes measured by Laurdan fluorescence spectroscopy."* DOI: 10.1016/j.bbamem.2021.183794

The Microbial Electrochemical Peltier Heat: Electroactive Microorganisms and Entropy Export

ID: 11058
09:25 - 09:50

Dr. Benjamin Korth[1]; Prof. Dr. Thomas Maskow[1]; Cornelia Dilßner[1]; Anne Kuchenbuch[1]; Dr. Matthias Schmidt[2]; Prof. Dr. Falk Harnisch[1]

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A fundamental principle of life is the coupling of the oxidation of an electron donor to the reduction of an electron acceptor, resulting in the formation of energy carriers for biomass formation. Microbial life evolved to exploit myriads of combinations of electron donors and acceptors, leading to entropy-driven (i.e., export of metabolic products with a higher entropy) and enthalpy-driven (i.e., export of heat) growth with many variants in between.

Electroactive microorganisms (EAM) represent a unique variation of these fundamental principles as they couple their metabolism to insoluble electron conductors. The underlying process is called extracellular electron transfer (EET) and allows the exchange of metabolic electrons with metal ores in nature or electrodes in technical systems. In an anodic scenario, EAM oxidize a soluble electron donor and transfer the released electrons to the anode, resulting in current flow. Based on the peculiarity of EET, the entropy export of EAM is fundamentally different compared to microorganisms utilizing soluble electron acceptors as it mainly relies on electron transfer and not the secretion of small molecules or dissipation of heat. During EET, the electron's state shifts. It changes from a restricted probability of presence within biomolecules to a completely delocalized state in solid electrodes. This state transition of the electrons means a significant increase in entropy accompanied by a reversible heat flux. This entropic effect at the interface EAM/electrode is called microbial electrochemical Peltier heat (mePh).

To investigate if the mePh is a material constant for biological systems, *Geobacter anodireducens* enrichment biofilms were cultivated at silver, gold, and copper electrodes. The heat fluxes were measured in a bioelectrocalorimetric setup by performing redox titration experiments. Furthermore, the contribution of the electrolyte to the heat flux was assessed by applying the entropy of transport concept.

Ultra Sensitive DSC Technologies – Thermodynamic Investigations and HTS of Protein Stability

ID: 12004
09:50 - 10:15

Marco Coletti[1]; Peter Vikegard[2]

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Differential scanning calorimeters (DSC) for studies of solute behaviour in liquid solvent was first developed in the 1960's with the purpose of investigating the behaviour of globular proteins as they unfold [1]. Thermodynamic investigations over the coming decades with this new technique led to deeper understanding of the stabilization of proteins e.g., phenomena like cold denaturation and the existence of a temperature at which a protein has its maximum stability. Hitherto the existence of cold denaturation had only been known on empirical basis [2]. A fundamental property that describes the energetics and stabilisation of proteins is the partial heat capacity, and especially how it changes as a protein unfolds, i.e. is transferred from its native state to a denatured state [3]. Continuous improvement in instrumentation has now reached a point at which the partial heat capacity of solutes in the $\mu\mathrm{g\,mL^{-1}}$ concentration range, diluted in aqueous media, can be detected.

With the advent and recent increase of proteins for various commercial purposes including clinical therapy, wild-type and genetically modified, has led to an increased interest from various industries in the technique. In this a more pragmatic view on how the technique is used has evolved, namely, to assess stability through the *thermostability*, often characterized by the denaturation or meltingtemperature, T_m, of a protein. Experimentally, such information is straightforward to obtain even in situations where irreversible aggregation might obscure accurate estimation of thermodynamic quantities such as the changes in enthalpy, and heat capacity. A general idea is that the higher the T_m, the higher is the conformational stability close to ambient condition which in turn leads to longer ßhelf-life". This idea has found multiple use in industry including activities such as formulation development, impact of genetic modification, batch-to-batch variability, and biosimilars [4,5].

In this contribution, the concept of *thermostability* and *thermodynamic stability* will be introduced and exemplified as well as recent developments of instrument, both for in-depth thermodynamic studies as well for high sample throughput screening of denaturation temperatures.

References:

1. P. Privalov and (1976) Methods in Enzymology, 131.
2. F. G. Hopkins (1930) Nature, 126.
3. J. Gómez et al (1995) Proteins, 22.
4. Olsen et al (2009) Thermochimica Acta 484.
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Day 3 | Block 2 - Oral Presentations

June 12th, 11:00 AM – 11:45 PM CEST

HALL A: Biophysical Chemistry (Chair: Thomas Maskow)

Invited Lecture:

ID: 12010
11:00 - 11:45

Computational Approaches to Microbial Energetics, Metabolism, and Growth

Prof. Dr. Ralf Steuer[1]

[1] *Universität Leipzig, Faculty of Physics and Earth System Sciences, Leipzig, Germany*

Microbial growth is governed by fundamental trade-offs in energy usage, resource allocation, and adaptation to environmental change. The talk will present computational approaches that help to quantify these trade-offs, from genome-scale constraint-based models to coarse-grained descriptions of cellular energetics. A particular focus is on phototrophic RoyalBlueobacteria, where light harvesting, photoinhibition, and variable quantum yields are integrated into flux balance models to predict growth and photosynthetic performance. The model predicts ATP and NADPH demands across cellular processes and reveals how cells allocate energy between biosynthesis, maintenance, and environmental sensing. We also explore how thermodynamic constraints and energy dissipation shape growth strategies in time-varying environments, where microbes must balance instantaneous growth with long-term fitness. We argue that strategies of cellular growth and resource allocation can be understood through the lens of thermodynamic efficiency and trade-offs. The results provide a quantitative basis for understanding microbial fitness beyond instantaneous growth, with implications for ecology and biotechnology.

Poster Presentations

June 11th, 14:45 PM – 15:45 PM
June 12th, 11:00 AM – 11:45 AM
June 12th, 14:20 PM – 15:00 PM
June 13th, 10:15 AM – 11:00 AM

Characterization of Components of PFS at Cryogenic Temperature by Thermal Analysis

ID: 10677
Poster Nr. A1

Dr. Angela Hammer[1]*; Nrec Nikolla*[1]*; Prof. Dr. Oliver Germershaus*[2]

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[2]*School of Life Sciences FHNW, Institute for Pharmatechnology and Biotechnology, Muttenz, Switzerland*

As the world transitions from the pandemic to an endemic phase of COVID-19, annual revaccination is recommended [1]. There are challenges with multidose vials due to their limited shelf life once opened. This has led to a shift towards pre-filled syringes (PFS), which offer benefits but also face technical difficulties, particularly with mRNA vaccines that require cryogenic storage (lower than $-70\,^{\circ}\mathrm{C}$) [2,3]. PFS consists of components like a needle shield, plunger (halogenated elastomers), and barrel (cyclic olefin polymer) [3,4]. A major challenge with PFS is the differing thermal expansion coefficients of these materials, which can affect the seal between the plunger and barrel under cryogenic conditions, risking contamination, leakage, and dosing inaccuracies [5].

In this contribution, syringe material (stopper and needle shield) were analyzed by DSC and TMA.

References:

1. M. Biancolella u. a., Hum. Genomics, Bd. 16, Nr. 1, S. 19, Dez. 2022
2. A. Badkar, A. Wolf, L. Bohack, und P. Kolhe, „, AAPS PharmSciTech, Bd. 12, Nr. 2, S. 564–572, Juni 2011
3. G. Sacha, J. A. Rogers, und R. L. Miller, Pharm. Dev. Technol., Bd. 20, Nr. 1, S. 1–11, Jan. 2015
4. C. Jansen-Otten und B. Zeiss, „All-About Prefilles Syringe Systems“, Venice, 21. April 2023
5. Z. Li u. a. Epidemiol. Infect., Bd. 149, S. e155, 2021

Calorimetric studies of interactions of non-wetting liquids with porous materials

ID: 10680
Poster Nr. A2

Prof. Dr. Mirosław Chorążewski[1]*; Dr. Alexander Rowland Lowe*[1]

[1] *University of Silesia, Faculty of Science and Technology, Katowice, Poland*

High-pressure scanning calorimetry otherwise known as Scanning Transitiometry can be used to characterize the thermomechanical properties of solid-liquid interface development. More explicitly it has been used to measure the heat and work of liquid intrusion into/from porous materials with a broad range of pore sizes. This is done through the simultaneous recording of three different variables which include, power, volume and pressure. Treatment of the power data provides the calorimeter curve which is used for calculating the heat of intrusion/extrusion which is combination of interface development and change in internal energy of water structure as it enters the porous structure. The work is calculated by combining the pressure and volume data to create pressure volume isotherms which can be used to determine the average pressure of filling/emptying, otherwise known as the intrusion/extrusion pressure. Simultaneously this allows us to identify the volume of intruded liquid, otherwise know as the intrusion volume. These values fundamentally describe the base energetics of the intrusion of water into the hydrophobic network, however they can fundamentally be adjusted through other means such as the addition of solutes or changing the crystallite size of the material. These parameters can be used to devise energy storage system, shock absorbers or bumpers.

Funding:
This project leading to this application has received funding from the European Union's Horizon 2020 research and innovation programme under Grant Agreement No. 101017858.

Method Development for Determining Water Adsorption Enthalpies in Confined Spaces with Varied Pore Wall Chemistry Using Differential Scanning Calorimetry

ID: 10814
Poster Nr. A3

Uta Sazama[1]; *Dr. Markus Hollering*[2]; *Stefan Lauterbach*[2]; *Philip Lenz*[3]; *Prof. Dr. Michael Fröba*[3]

[1] *University of Hamburg, Institut für Anorganische und Angewandte Chemie, Hamburg, Germany*
[2] *NETZSCH-Gerätebau GmbH, Selb, Germany*
[3] *University of Hamburg, CUI: Advanced Imaging of Matter, Hamburg, Germany*

Understanding the behavior of water on surfaces and within confined pore spaces is crucial in various fields, including biochemistry—where water interacts with cell membranes—and in catalysis and energy storage.
Previous studies using differential scanning calorimetry (DSC) have shown that nanoconfinement of water significantly lowers its freezing and melting points. [1,2] To gain deeper insight into the interplay between pore size, surface chemistry, and the interfacial behavior of confined water, further investigation of water vapor adsorption and condensation in pores of varying size and surface hydrophilicity is required. For this purpose, a humidity attachment for the NETZSCH DSC 300 Caliris® Classic was developed in cooperation with Netzsch. The desired humidity is introduced directly into the measurement chamber via a humidity generator. A fixed adjustment of the humidity chamber and carrier gas flow ensures a consistent distance between the sample and reference in the heat flow calorimeter.
DSC experiments were conducted to determine water vapor adsorption enthalpies on various mesoporous silica materials (e.g. MCM-41 type) at $298\,\mathrm{K}$ and under varying relative humidity. These results were validated by simultaneous thermogravimetric differential scanning calorimetry (TGA-DSC) experiments on the same samples.

References:

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2. J. B. Mietner, F. J. Brieler, Y. J. Lee, M. Fröba, Angew. Chem., Int. Ed. (2017), 56, 12348 -12371

Investigation of Redox Reactions of Redox-Active and Thermoresponsive Polymers Using Isothermal Titration Calorimetry

ID: 10821
Poster Nr. A4

Annika Böhle[1]; Bianca Störr[1]; Annika Lehmann[1]; Dr. Erik Schumann[1]; Dr. Konrad Burkmann[1]; Dr. Andreas Lißner[1]; Marvin Schmieder[1]; Prof. Dr. Felix Plamper[1]; Prof. Dr. Florian Mertens[1]

[1]Technische Universität Bergakademie Freiberg, Faculty of Chemistry, Physics and Biosciences, Institute of Physical Chemistry, Freiberg, Germany

Redox-active microgels based on thermoresponsive poly(N-isopropylacrylamide) (P(NIPAM)) have emerged as a promising class of active compounds for energy storage applications.[1–3] Our research aims to deepen the understanding of charge transfer processes influenced by the architecture of the polymer. We systematically compare microgels with redox-active groups to their elemental electroactive group and linear polymer counterparts. Microgels and linear P(NIPAM) polymers with varying chain lengths have been modified with various redox-active groups, including viologen, TEMPO, and ferrocene derivatives. The impact of these modifications on the thermoresponsive behavior of the polymers in aqueous solutions has been examined using a Micro DSC IIIa (Setaram). The energy which is released during redox reactions between differently charged electroactive groups should be measured in terms of heat using isothermal titration calorimetry (ITC). For this purpose, a Thermometric 2277 Thermal Activity Monitor (TAM) is used. Conducting these measurements under oxygen-free conditions is crucial, as some reduced species are highly sensitive to oxidation by oxygen. To establish these conditions, the titration ampoule is flushed with nitrogen prior to measurement, and a nitrogen bypass is incorporated to ensure the measurement cell remains oxygen-free while enabling pressure exchange during the measurement.

References:

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3. E. Y. Kozhunova, A. I. Inozemtseva, M. A. Nazarov, A. D. Nikolenko, E. S. Zhvanskaya, O. I. Kiselyova, M. V. Motyakin, S. V. Kutyakov, A. A. Pakhomov, D. M. Itkis, A. V. Chertovich, A. R. Khokhlov, Electrochim Acta 2024, 475, 143534.

Application of nanoITC in the analysis of the interaction between newly synthesized substances with potential anticancer activity and DNA. Preliminary study.

ID: 10847
Poster Nr. A5

Aleksandra Owczarzy[1]*; Dr. Wojciech Rogóż*[1]*; Karolina Kulig*[1]*; Prof. Andrzej Zięba*[1]*; Prof. Małgorzata Maciążek-Jurczyk*[1]

[1] *Medical University of Silesia, Department of Physical Pharmacy, Katowice, Poland*

Cancer treatment is one of the challenges of modern medicine. The advancement of new anticancer drugs requires a comprehensive understanding of their mechanism of action. Binding of small molecules to DNA can inhibit or modify cellular DNA function and induces cell death. 9-Fluoro-5-alkyl-12(H)-quino[3,4-b][1,4]benzothiazinium chloride (Salt2) are newly synthesized substances with potential anticancer activity. Salt2 has been tested in vitro against the HCT116 and LLC tumor cell lines versus doxorubicin.

The recorded nanoITC thermograms and binding isotherms show that Salt2 can form a complex with ctDNA. Experimental data showed that the enthalpy (ΔH) and entropy (ΔS) changes were positive, while the Gibbs free energy (ΔG) change was negative, and the binding stoichiometry oscillated around 1. The obtained mean K_a value indicates that Salt2 binds to ctDNA with moderate affinity, which is ideal from an experimental point of view, because binding affinity, thermodynamic parameters and stoichiometry can be determined independently in a single experiment without any assumptions.

The negative values of ΔG illustrated that Salt2-ctDNA complex formation is a spontaneous, entropy driven endothermic process with positive enthalpy and entropy changes. In addition, the positive values of ΔH and ΔS may suggest that the non-covalent interactions (hydrogen bonds, van der Waals force, hydrophobic interactions) may be involved in the studied complex formation.

Acknowledgement: This work was supported by Grants BNW-2-048/K/4/F, BNW-1-009/K/4/F, BNW-2-049/K/4/F and BNW-2-110/K/4/F from the Medical University of Silesia, Poland.

Calorimetry and thermal analysis of solid-state batteries

ID: 10861
Poster Nr. A6

Dirk Florian Hunstock[1]*; Dr. Alexander Sedykh*[1]*; Prof. Dr. Maren Lepple*[1]

[1] *Justus Liebig University Giessen, Institute of Inorganic and Analytical Chemistry, Giessen, Germany*

Safety evaluation of batteries plays a crucial role in the development of next generation systems. With an expanding electrochemical window, the Gibbs energy of materials used increases and, therefore, simultaneously raises the potential hazards in case of a thermal runaway and other failing mechanisms. Transition to solid state batteries (SSBs) should improve thermal safety as well as energy density in comparison to conventional Li ion batteries with liquid electrolyte. Nonetheless, actual measurements and definition of thermal properties of SSBs and their constituent materials are necessary. Numerous analysis methods are employed to characterize the thermal properties of battery materials, including their fundamental thermochemical quantities. Drop solution (DS) calorimetry is used to determine enthalpies of dissolution of battery materials. For oxidizable compounds (sulfide based electrolytes) combustion calorimetry is used to determine their enthalpy of combustion. In combination with an adequate thermochemical cycle, it is possible to obtain other meaningful thermochemical quantities, such as enthalpies of formation, for all components of SSBs using these two calorimetric techniques. Simultaneous thermogravimetry and differential scanning calorimetry (TG DSC) are used for investigation of thermal stability of compounds and composite materials and investigation of battery venting events. In addition, the heat generation of whole cells can be investigated. Coupling calorimetry with battery cycling experiments connects common battery data quantitatively with the heat signature of underlying processes.

Additional thermodynamic and thermophysical quantities, such as coefficient of thermal expansion (CTE) measured by dilatometry or temperature-dependent X ray diffraction, specific heat capacity CP obtained from DSC data, and thermal conductivity of ceramics assessed by laser flash analysis (LFA), can enhance the understanding of processes in solid state batteries.

Thermal Behavior and Energy Content of Soil Organic Matter Building Blocks: Insights from Simultaneous Thermal Analysis

ID: 10880
Poster Nr. A7

Prof. Dr. Christian Fricke[1,5]; Dr. Marcel Lorenz[2];Prof. Dr. Thomas Maskow[3]; Prof. Dr. Sören Thiele-Bruhn[2]; Prof. Dr. Monika Normant-Saremba[4]; Prof. Dr. Gabriele Ellen Schaumann[5]

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[5]*University of Kaiserslautern-Landau, Department of Natural and Environmental Sciences, Environmental and Soil Chemistry Lab, Landau, Germany*

Chemical energy from carbon sources like plant and animal debris fuels microbial activity and matter exchange in soils. Soil organic matter (SOM) plays a key role in storing, regulating, and transforming carbon and energy. SOM comprises a wide variety of molecular building blocks with different energy contents and structural complexities, ranging from simple sugars to complex peptides, lipids, and condensed polyaromatic compounds. These differences complicate the thermodynamic characterization of SOM and the precise determination of its energy content—crucial for understanding SOM turnover and stabilization.

This study applies a bottom-up approach to examine thermal reactions of 13 SOM building blocks and source materials (e.g., glucose, cellulose, chitin, plant litter, fungal/bacterial necromass) using simultaneous thermogravimetry (TG) and differential scanning calorimetry (DSC). A quadrupole mass spectrometer (QMS) monitored evolved gases during combustion. The temperature range for energy determination was based on the CO_2 signal (44 m/z) from QMS for each compound. Energy contents derived from TG-DSC-QMS were compared with results from conventional combustion calorimetry.

Findings show energy contents from $7\,\mathrm{kJ\,g^{-1}}$ OM for carbohydrates to $22\,\mathrm{kJ\,g^{-1}}$ OM for bacterial necromass, with notable deviations from combustion calorimetry values. The DSC combustion patterns reflect SOM bond energetics: weak bonds (e.g., in carbohydrates) yield an exothermic peak below $400\,^{\circ}\mathrm{C}$ (exo1), while strong bonds (e.g., in peptides, polyaromatics) produce peaks above $400\,^{\circ}\mathrm{C}$ (exo2). QMS data also show that char from exo1 compounds contributes to exo2 peaks.

In summary, TG-DSC-QMS improves our understanding of SOM combustion behavior and offers a more nuanced view of SOM energetics compared to traditional methods. Future studies should explore interactions between SOM and soil minerals to better interpret energy contents of natural soil OM.

Contribution of minerals and organic material to the energetic signatures of soil – Insights from an artificial soil experiment and calorimetric analyses

ID: 12007
Poster Nr. A8

Dr. Marcel Lorenz[1, 2]*;Prof. Dr. Christian Fricke*[3]*; Dr. Tobias Bölscher*[4]*; Dr. Klaus Kaiser*[5]*; Prof. Dr. Thomas Maskow*[2]*, Prof. Dr. Sören Thiele-Bruhn*[1]

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[5] *Martin Luther University Halle-Wittenberg, Institute of Agricultural and Nutritional Sciences, Halle (Saale), Germany*

The thermodynamic perspective on soil systems is receiving increasing attention and has the potential to contribute to a holistic understanding of soil organic matter (SOM) dynamics. An integral part of new bioenergetic concepts is the energy content of SOM, but its determination particularly in mineral soils is challenging. A promising technique in this respect is thermogravimetry combined with differential scanning calorimetry (TG-DSC). Here, the heat flow and mass losses are measured simultaneously in a controlled combustion of the soil material during a temperature increase from 50 to 1000°C under an oxidative atmosphere. Heat and mass changes in the range of 180-600°C are usually interpreted as the result from the exothermic combustion reaction of SOM and thus used to derive the energy content (combustion enthalpy, $\Delta_C H$) of SOM. Overlapping exo- and endothermic reactions by other non-oxidizing processes (e.g. dehydroxylation/-carboxylation and desorption of soil minerals) in that temperature range are often neglected because their quantification and differentiation from the rather strong exothermic oxidation reactions of SOM is challenging.

To disentangle these reactions, we determined the $\Delta_C H$ of cellulose as model substrate for SOM and additional soil minerals (quartz sand, quartz silt, goethite, illite, montmorillonite) 1) individually, 2) intensively mixed in the dry state, and 3) intensively mixed after several wetting-drying cycles. The minerals were mixed to create a silt loam texture and combined with cellulose to mimic a soil. Calorimetric analyses were conducted using a TG-DSC coupled with a mass spectrometer to analyze the gases (H_2O, CO_2) evolved during combustion.

First results show that the $\Delta_C H$ value obtained by TG-DSC is lower for cellulose to reference values obtained by combustion calorimetry as the standard method. Furthermore, $\Delta_C H$ differs when mineral compounds are mixed with cellulose, indicating that thermal reactions by mineral compounds affect the determination of the energy content by TG-DSC. This is supported by the analyses of the pure minerals, which revealed exothermic and/or endothermic side reactions for all minerals in the range from 180-600°C affecting the TG-DSC signal. Depending on the mineral composition of the soil, the energy content of SOM can be substantially over- or underestimated by TG-DSC. This is particularly important for soils rich in oxides and clay minerals.

In the next step we want to derive the thermal activation energy (E_a) from the thermograms, which represents the energy required to initiate the combustion of SOM. In other studies, the ratio of $\Delta_C H/E_a$ was conceptualized as the return on (energy) investment"(ROI), a proxy to evaluate the microbial degradability of OM. Yet, the influence of thermal reactions by mineral soils on Ea remains largely unknown. Building on the findings of our artificial soil experiment, we aim to provide methodological considerations for the use of TG-DSC in the energetic characterization of SOM. This will take into account the contribution of mineral oxidation and the effect of organo-mineral associations on the energy content and E_a. This is crucial if energy fluxes and sinks in soil systems are to be quantified to better understand OM turnover and stabilization in soil.

Step-wise dissolution DSC analysis as a tool in the development of partially soluble API/polymer systems for individualized medicine

ID: 11025
Poster Nr. A9

Johannes Lang[1]*; Dr. Jan Henrik Finke*[1]

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3D printing is a promising tool for the paradigm shift from industrial mass production to patient-tailored dosage forms due to its flexibility and ease in individualizing doses and release profiles. Fused deposition modelling (FDM) is currently the most extensively researched 3D printing approach in the pharmaceutical context. A critical step in this process is the preparation of the active pharmaceutical ingredient (API)-loaded filaments, which is primarily done using hot-melt extrusion (HME). These polymer composite filaments can be formulated to form amorphous solid dispersions (ASDs) in which the API is molecularly dispersed in the polymer matrix. In this case, the API's temperature-dependent solubility in polymer matrices and the resulting risk of uncontrolled recrystallization upon cooling and storage limit the maximum API concentration thus also restricting dose flexibility during 3D printing. An alternative strategy is to develop filaments with API concentrations that exceed their solubility in the polymer matrix also at processing temperature. This results in residual particles throughout the process chain that act as crystallization nuclei on cooling, allowing controlled recrystallization. In this study, the step-wise dissolution DSC method is used to generate phase diagrams of API/polymer systems. From these, process windows in terms of minimum and maximum API concentration at given process temperatures (HME and 3D printing) are derived, that secure a binary system with particulate API throughout the whole process chain. Several challenges arose from the pharmaceutical excipients and APIs studied, including the non-assessability of glass transition temperatures and decomposition during melting. Strategies to overcome these hurdles are presented, comprising extrapolation of properties by alternative binary blend partners and new thermoanalytical approaches to cope with decomposition.

Flash calorimetric investigation of Ni/Al multilayer thin films: Ultra-high heating rates kinetics.

ID: 11034
Poster Nr. B1

Dr. Andrey Tarasov[1]

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Ni/Al multilayer thin films, characterised by macro- and nanoscale morphologies, are of great interest due to their high interface density and stored chemical energy. Most research has focused on slow heating in the solid state or ignition processes after thermal or mechanical shock. In these scenarios, the films act as localised heat sources, allowing room-temperature soldering of materials with different thermal expansion coefficients.

There is a notable lack of data on intermediate and ultra-fast heating rates, with only a few advanced in-situ measurements available. This study used the Mettler-Toledo FDSC 2+ for calorimetric measurements at heating rates up to $10\,000\,\mathrm{K\,s^{-1}}$, alongside conventional DSC experiments. The resulting dataset enables model-based kinetic analysis of rapid heating rates to explore the connection of various exothermic events such as interdiffusion and intermetallic phase formation.

We investigated the Ni/Al multilayers with $5\,\mathrm{\mu m}$ thickness, overall composition of $Ni_{50}Al_{50}$ at. % and a bilayer periodicity (Λ) of $20\,\mathrm{nm}$.

FDSC scan at $500\,\mathrm{K\,s^{-1}}$ with its deconvoluted fitting curve highlights distinct peaks for different intermetallic phases in agreement with reaction thermodynamics. The reaction follows consecutive kinetics with activation energies between 180-210$\mathrm{kJ\,mol^{-1}}$ (ca. $2\,\mathrm{eV}$) up to $5000\,\mathrm{K\,s^{-1}}$. The maximum reaction rate, represented by heat flow, occurs at this heating rate, merging multiple steps into a single peak. Two of the five steps exhibit similar reaction rates, and their intermediate product concentrations approach zero at higher rates. Our study reveals a multistep reaction mechanism not previously modelled at flash heating rates.

This observation utilised advanced calorimetric methods on multilayers, expanding data analysis to intermediate and flash rates. We validated our results with microstructural analyses like XRD and TEM.

Safety First: Calorimetric Evaluation of VC and FEC Additives in Lithium-Ion Batteries and Their Impact on Performance

ID: 11060
Poster Nr. B2

Karsten Geuder[1]; Prof. Dr. Hans Jürgen Seifert[1]; Dr. Carlos Ziebert[1]

[1] Karlsruhe Institute of Technology (KIT), Institute for Applied Materials - Applied Materials Physics, Department Composites and Thin Films, Eggenstein-Leopoldshafen, Germany

The safety of lithium-ion batteries is a key concern in their widespread adoption across consumer electronics, electric vehicles, and stationary storage. Thermal runaway remains one of the most critical challenges, making it essential to understand and control heat-generating reactions within the cell. Calorimetry offers a powerful toolbox to investigate thermal behavior from materials to full-cell systems.

Dry cells were assembled with a baseline electrolyte (EC:EMC 3:7, $1\,\mathrm{M}$ $\mathrm{LiPF_6}$), with or without 5 wt% VC or FEC. The cells, based on NMC622/graphite electrodes, demonstrated stable capacities $>1\,\mathrm{A\,h}$. The decomposition of additive containing electrolyte occurred earlier than the base electrolyte ($2.4\,\mathrm{V}$ for VC, $2.6\,\mathrm{V}$ for FEC vs. $\sim 2.8\,\mathrm{V}$ without additives), aiding in the formation of a more stable solid electrolyte interphase (SEI).

This study explores the safety effects of two commonly used electrolyte additives, vinylene carbonate (VC) and fluoroethylene carbonate (FEC), using a combination of calorimetric techniques. Differential Scanning Calorimetry (DSC) was used to assess the thermal stability of the separator, showing melting onset at $119\,^{\circ}\mathrm{C}$, typical for polyolefin-based separators. The thermal behavior of the individual electrodes combined with electrolyte was analyzed via highly sensitive Tian-Calvet microcalorimetry in the temperature range of $30\,^{\circ}\mathrm{C}$ bis $300\,^{\circ}\mathrm{C}$. Full-cell thermal safety was evaluated using the Heat-Wait-Seek method in an Accelerating Rate Calorimeter (ES-ARC), providing a comprehensive understanding of exothermic behavior during thermal abuse. Exothermal onset was found at around $135\,^{\circ}\mathrm{C}$ for all tested electrolyte variations. A temperature rate of $9\,^{\circ}\mathrm{C\,min^{-1}}$ was used as indication for the start of cell´s thermal runaway. It was observed between $220\,^{\circ}\mathrm{C}$ bis $230\,^{\circ}\mathrm{C}$.

Future work will extend this approach to aged cells, aiming to understand long-term safety implications.

Venues / Locations

Conference Venue, Wednesday June 11 - Friday June 13

Leipziger KUBUS
Helmholtz-Centre for Environmental Research – UFZ
Permoserstraße 15 | 04318 Leipzig

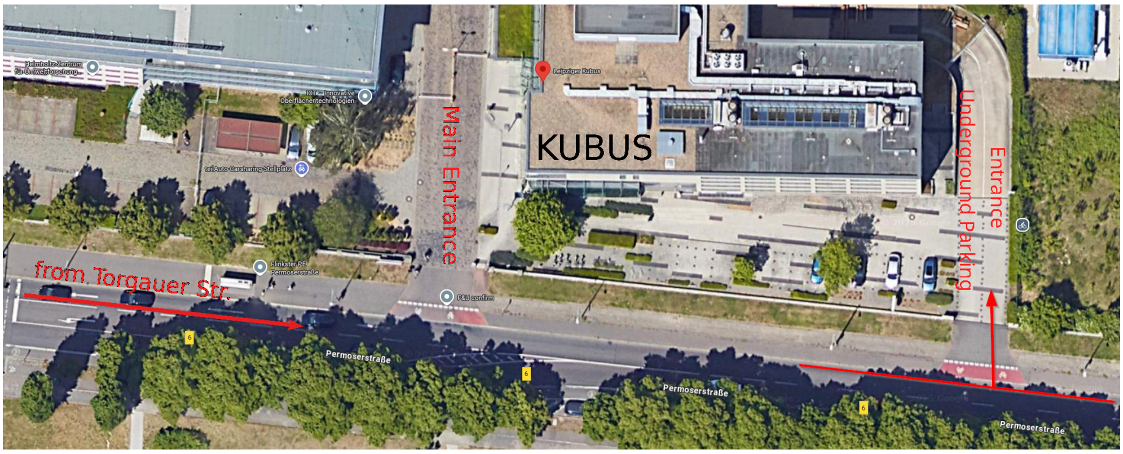
Oral Presentations: Hall A and Hall B (First floor)

Poster Presentations: Foyer (Ground floor)

Exibitions: Foyer

How to get there:
By public transport: From Leipzig main station, take tram line 3 (direction *Sommerfeld* or *Taucha*) to the *Torgauer/Permoserstraße* stop, then walk into *Permoserstraße*. After approx. 300 meters you will find the *KUBUS* on the left. Travel time approx. 15 minutes.

By car: From A14 motorway, take the exit *Leipzig-Nordost*. Follow signs to *Stadtzentrum* via *B87/ Torgauer Straße*. After about 3.5km turn left into *Permoserstraße*. After another 250m you find the entrance to the UFZ site on the left.
For parking, please do not take the main entrance to the UFZ site but rather the second driveway, 50 meters further down the road, directly into the underground car park.



Get-Together at Cafe Madrid, Wednesday evening

Wednesday, June 11, from 7:00pm
Informal social gathering for dinner and drinks on self-pay basis
—
Cafe Madrid (Restaurant - Tapas - Bar)
Klostergasse 3-5 | 04109 Leipzig
https://www.cafe-madrid.de/

How to get there:
From the *KUBUS* walk to tram station *Torgauer/Permoserstraße*, take tram line 3 (direction *Grünau*) to the *Goerdlerring* stop (one stop after main station), then walk into *Hainstraße* to the city center's market square. Turn into *Barfußgässchen*, then left into *Klostergasse*. Travel time approx. 30 minutes.

Guided City Tour and Conference Dinner, Thursday evening

Guided City Tour: Thursday, June 12, 5:30pm to 6:30pm
Starting at: Katharinenstraße 8
Guided Tour ends at Auerbachs Keller
—
Conference Dinner - Auerbachs Keller:
Thursday, June 12, from 6:30pm
Grimmasche Straße 2-4
https://www.auerbachs-keller-leipzig.de/

How to get to the City Tour:
From the *KUBUS* walk to tram station *Torgauer/Permoserstraße*, take tram line 3 (direction *Grünau*) to the main station (city center), then cross the road and walk towards city center to *Nikolaistraße*. After about 150m turn right into *Brühl*. Follow *Brühl* for about 200m, then turn left into *Katharinenstraße*. Travel time approx. 30 minutes.

Historical tour:
A walk through the compact city with the tour guides is the best way to get to know the famous sights of Leipzig city center in a short time.

Many topics relevant to Leipzig are covered: Trade fair architecture with arcades, St. Thomas' and St. Nicholas' Churches, the peaceful revolution in the autumn of '89, Leipzig as a city of music, writers in Leipzig, Auerbach's Keller and much more.

Leipzig, the city of music - tour:
Whether Johann Sebastian Bach, who took up the post of Thomaskantor in 1723 and directed the now world-famous Thomanerchor, or Georg Philipp Telemann, who celebrated his first major compositional successes here, whether Robert Schumann, who discovered his love for Clara Wieck here, or Felix Mendelssohn Bartholdy, who worked as Gewandhauskapellmeister and founded a conservatory to train his musicians, or Richard Wagner, Albert Lortzing, Gustav Mahler and others - musical Leipzig has many facets, which are explored on this stimulating tour.

How to find Auerbach's Keller:
Located at the southern end of the central market square within the *Mädler-Passage*