

Illustration of an artificial skin model obtained by 3D printing viewed by optical microscopy.

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### **Preface**

Two years ago, I thought that ChatGPT did not need to be mentioned in the ICP annual report because we do not do Large Language Model (LLM) research. Last year, however, it seemed worth mentioning as a topic and I outlined a vision for applications in the field of software tools for physical simulation [1]. I would now like to return to the topic and report on the use of the new tool in teaching. We have challenges and interesting new use cases for both lecturers and students.

In teaching, a profound change due to the existence of LLMs can be recognised in tasks where students have to submit a report. It is undisputed that developing thoughts and formulating them in words is an important mental activity for students that promotes the learning process. If we stick to the report form as before, the brain activity will no longer be a creative activity, but rather a passive (at best critical) counter-reading of texts generated by ChatGPT. Instead of writing a report, however, the LLM can enter into an interactive dialogue with students and follow their thoughts. The dialogue encourages students to think for themselves and removes a barrier, especially for the more introvert or shy students. A concrete example: in preparation for the end-of-semester oral exam in physics, I provided students with a customised chatbot that formulates questions and receives answers. These are voluntary learning units to simulate the oral exam. I am then present in the practice sessions, and I am offering something more than the LLM with solving oral exercises at the blackboard. The discussions are stimulating, because you get direct student feedback in a personal exchange, can be directly present at some of the *aha* moments and recognise the real hurdles in the subject better.

Interested in this digital mentor? The tool is available free of charge within the ZHAW [2]. It was funded by the Transformative Educational Fund [3] and programmed by Kurt Pernstich. It is currently being used in a beta test version in some places. The tool allows lecturers to create new digital assistants which are instructed in normal language about the scope of the subject and their specific tasks in dialogue with the students. A corresponding tutorial is included in the tool. We are looking forward to your feedback.

I now recommend that you continue reading the short reports on ICP's research projects. I would like to thank the entire ICP team, on the one hand for their great commitment, but at least as much for the pleasant working atmosphere and the inspiration.

Andreas Witzig, Head of ICP

#### Links:

- [1] https://www.zhaw.ch/de/engineering/institute-zentren/icp/forschungsberichte
- [2] https://mentormate.zhaw.ch
- [3] https://www.zhaw.ch/en/focus-topics/zhaw-digital/education/tef

## 1 Multiphysics Modeling

Multiphysics modeling is a powerful tool for exploring a wide range of phenomena, coupling flow, structure, electro-magnetic, thermodynamic, chemical and/or acoustic effects. The past decades have been a period of rapid progress in this area. In fact, the possible range of applications has been widely expanded and numerical methods have become increasingly sophisticated and adapted to exploit available computational resources. Today, detailed physical-chemical models combined with robust numerical solution methods are almost a necessity for the design and optimization of multifunctional technical devices and processes.

At the ICP, we perform applied research in the field of multiphysics modeling and develop finite element as well as finite volume simulation software. Our extensive experience in numerical analysis, modeling and simulation allows us to successfully apply simulation-based optimization in many fields. We are familiar with a wide range of governing physical equations and find numerical solutions even when the effects are closely interrelated. We also develop single-purpose numerical tools tailored to the specific needs of our partners, and we use commercial software where it is more suitable. Our specialties in this context include the application, extension and development of coupled models using our own finite element software SESES, the fluid dynamics software OpenFoam (open source) and commercially available products such as COMSOL.



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S. Ehrat

# 1.1 Thermal Design Lab - Determining the thermophysical properties of liquids and solids

In our R&E projects, we support our project partners with physical computer simulations. Their accuracy requires reliable material data, which is often not available in the literature and therefore requires our own measurements.

Contributors: S. Ehrat, G. Martins Marcello, T. Hocker Partners: Medyria AG, Universitätsspital Zürich (USZ)

Funding: ICP, Innosuisse Duration: Fortlaufend

Various measuring instruments are available in the Thermal Design Lab to analyze the thermophysical properties of liquids. The density of a liquid can be determined with the portable density meter "DMA 35" from Anton Paar, while the rotational viscometer "ViscoQC 300L" is used to specify the viscosity.

For thermal conductivity and specific heat, an excellent instrument for measuring thermophysical properties was recently acquired in the form of the "MP-V" from Thermtest. This versatile measuring platform can be equipped with different sensors to determine the thermal conductivity of solids, liquids, pastes and powders. The transient measuring principle is based on the time-dependent T-curve of the heating process by a constant heat source. This allows short measuring times and therefore an excellent measuring throughput. In addition, different modules in the measurement software allow the measurement of thin-film or anisotropic materials.

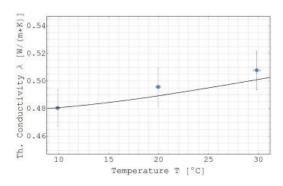


Fig. 1: Thermal conductivity measurement "S34" (sucrose-water) with measurement inaccuracy  $(3\sigma)$  compared to the literature values [1].

Different sugar and glycerine-water solutions were measured in order to evaluate the measurement procedure for the different instruments and to assess their accuracy against literature values. The figures show the measurement results (blue dots) for the heat transfer properties of a 33.72 M% sucrose-water mixture compared with the literature values (black line) [1][2].

After an additional correction of the measured data, which is carried out via a reference measurement with a model substance, the measured data show perfect agreement with the respective literature values. This applies to all sugar-water and glycerine-water mixtures that were analysed. Furthermore, the densities and dynamic viscosities were checked, which also show excellent agreement with the literature.

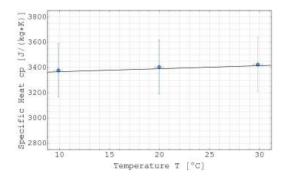


Fig. 1: Heat capacity measurement "S34" (sucrose-water) with measurement inaccuracy  $(3\sigma)$  compared to the literature values [1].

In addition to liquids, the MP-V can also be used to measure solids and thin-film materials. The required sensors and software licences are available for this purpose.

#### Literature:

[1] Ferenc A. Mohos, *Confectionery and Chocolate Engineering: Principles and Applications, 2nd Edition*, John Wiley & Sons, 2017.

[2] Mosen Asadi PhD, *Beet-Sugar Handbook*, John Wiley & Sons, 2005.

#### 1.2 Corrosion of multiphasic titanium alloy implants

Titanium alloys are frequently used for implants in the human body. Despite the excellent corrosion resistance of these alloys, oxidizing species produced during inflammatory episodes can lead to a corrosive attack. In this project, a Swiss/French consortium will reveal the basic mechanisms of the corrosion of additive manufactured titanium implants using a combination of experimental methods and mathematical modelling.

P. Marmet, Y. Safa, L. Holzer

Partners: Thermomechical Metalurgy Lab (EPFL), Institut de la Corrosion Brest France,

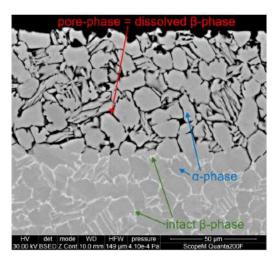
Laboratoire de Réactivité de Surface Sorbonne France

Funding: SNSF, French National Research Agency

Duration: 2023-2026

Titanium and its alloys are among the most widely used biocompatible materials as implants in the human body. However, they may deteriorate under the influence of several electrochemical, mechanical and biological factors. The corrosion resistance of titanium is mainly attributed to the presence of a thin passive layer on its surface, but this layer degrades in the presence of oxidizing species produced during inflammatory episodes, such as hydrogen peroxide or radicals that alter the passive film, leading to corrosion of the metal. In this project, a consortium of partners from France and Switzerland works together to reveal the basic mechanisms of the corrosion of additive manufactured Ti6Al4V implants using a combination of experimental methods and modelling. Fig. 1 presents the cross-section of a corroded Ti6Al4V sample after exposure to a PBS solution containing 3 % hydrogen peroxide for 10 days. A uniform dissolution of the  $\beta$ -phase is observed, extending to a depth of approximately  $70 \, \mu \mathrm{m}$ . To interpret the electrochemical corrosion experiments, the corresponding impedance spectra are modeled using Fig. 1: Cross-section of a corroded Ti6Al4V sample.

the actual geometry of the  $\beta$ -phase, reconstructed from FIB-SEM tomography (Fig. 2a, b). These structural data serve as the basis for frequencydomain simulations performed within Comsol Multiphysics (Fig. 2c, d), enabling the identification of microstructural influences on the electrochemical measurements (e.g., de Levie impedance feature).



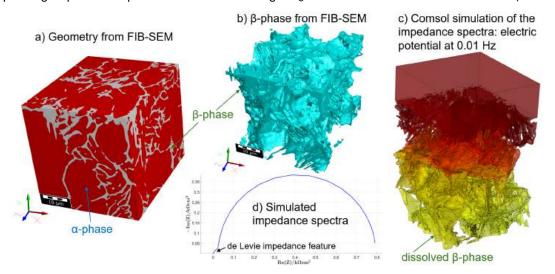


Fig. 2: Simulation of the electrochemical impedance spectra: a) and b) 3D Geometry from FIB-SEM tomography, c) and d) FEM frequency-domain simulation in Comsol Multiphysics.

### 1.3 Digital Wolfram - A real time TIG welding expert system

In a highly interdisciplinary team we are developing Digital Wolfram (DW), a TIG-welding expert system built on in-house hardware and software. It analyses voltage, current, arc-length and optical-emission signals to detect process anomalies in real time.

Contributors: T. Hocker, L. Holzer, D. Meier, M. Schmid, C. Fiant, R. Gubler, M. Abegglen,

J. Rosset, O. Hoenecke (ISC), A. Kipka, M. Türkes (BFH)

Partners: Wolfram Industrie GmbH

Funding: Innosuisse Duration: 2023–2025

Achieving top-quality TIG (Tungsten Inert Gas) welds requires a perfectly stable process. Undesired events—such as poor arc ignition or shielding-gas turbulences—can produce severe defects and force expensive, time-consuming rework. A digital assistant that warns welders about process instability therefore offers clear economic and quality benefits.

The heart of Digital Wolfram is a robust logger developed at the Institute of Signal Processing (ISC). Its galvanically isolated front end withstands the several-kilovolt spikes of contact-less ignition and streams 16 analogue and 12 digital channels at up to 40 kHz (Fig.1)



Fig. 1: Prototype of the Digital Wolfram logger in its rugged metallic housing.

Using this hardware we study how anomalies appear in voltage, current, arc length and optical emission data. To date, the system recognises more than twenty characteristic features. Some are straightforward process metrics, such as the given parameters of a pulsed-current welding signal. These values are essential for weld documentation. Other features point to disturbances that can trigger costly defects as for example bad arc starts or insufficient shielding gas coverage.

The user interaction is a key ability of such an expert system. Real time algorithms turn those detected anomalies into color-coded messages and alerts in a graphical user interface (see Fig. 2).

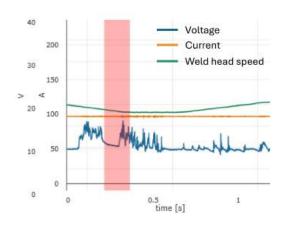


Fig. 2: Live GUI screenshot with voltage, current and weldhead velocity plotted against time. The anomaly-detection algorithm highlights a detected shielding-gas turbulence as a red translucent band.

The prototype has attracted strong interest from leading industrial players. Some of them are already beta-testing the system in research or production.

In the final project year, we will collect synchronised data from an even broader sensor collection and complement it with weld seam quality analyses (e.g. optical microscopy) and SEM images of electrode degradation. This will help deepen our understanding of cross-signal correlations and the underlying physics, such as electrode degradation mechanisms.

### 1.4 Digital Wolfram – Optical Emission Spectroscopy for Plasma Insight

Within the Digital Wolfram project we expand our TIG welding expert system beyond electrical sensors and analyse the emission of the TIG arc itself. By analysing optical emission spectra we estimate plasma temperature, electron density and species composition thereby addressing a critical gap in process control.

Contributors: T. Hocker, L. Holzer, D. Meier, M. Schmid, C. Fiant, R. Gubler, M. Abegglen,

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Partners: Wolfram Industrie GmbH

Funding: Innosuisse Duration: 2023–2025

Tungsten Inert Gas (TIG) welding employs an electric arc (Fig. 1) between a non-consumable tungsten electrode and the workpiece. An inert shielding gas — usually argon or helium — protects both the molten pool and the glowing electrode. The arc reaches roughly nine to twelve thousand degrees Celsius, ionising the shielding gas and metal vapour to form a plasma.

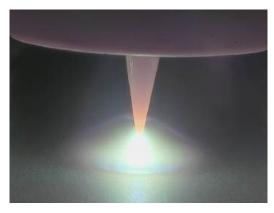


Fig. 1: Detailed view of the tungsten electrode and arc plasma during TIG welding with argon as the shielding gas.

Owing to its high seam quality, TIG welding is the method of choice in aerospace, nuclear technology and other technically demanding applications. Achieving that quality requires a stable, wellobserved process. Undesired process anomalies can lead to severe and costly defects. To gain more control over the process, we develop a digital assistant which warns the welder about such process instabilities, using algorithms primarily derived from current and voltage data. However, monitoring electrical data alone leaves an important blind spot: the composition and temperature of the plasma. Direct measurement is difficult, yet these quantities govern arc behaviour and in turn weld quality.

To fill this gap we collect time-resolved optical emission spectra using a fibre-coupled spectrometer. A custom-developed workflow generates a synthetic reference spectrum from spectroscopic constants, aligns its dominant lines with the measured spectra and then applies a multielement Saha–Boltzmann analysis to derive plasma temperature and the species composition. These parameters serve as indicators of process stability and help reveal critical faults — for example, when excess oxygen reaches the electrode.

Over the course of this year, we will validate the method using a broader dataset. Furthermore, we aim to integrate the key plasma indicators into a real-time algorithm, allowing them to appear alongside electrical warnings in the user interface.

### 1.5 Toward a corrosion mechanism model of titanium implant

Corrosion of titanium medical implant is often attributed to inflammatory effects in the human body affecting the life quality of considerable number of persons. Understanding the mechanism of the corrosive degradation of titanium implant helps for a better material design extending the implant durability. A model-based approach is adopted for a consistent analysis of corrosive activities in-between titanium alloy phases.

Contributors: Y. Safa, P. Marmet, L. Holzer

Partners: Mechanical Metallurgy Lab EPFL, Institut de la Corrosion Brest France,

Laboratoire de Réactivité de Surface Sorbonne France

Funding: SNSF, French National Research Agency

Duration: 2023-2026

Titanium is often considered as successful material option in the fabrication of medical implant for the human body. Titanium alloy (Ti6Al4V) includes  $\beta$  phase that provides special mechanical functionality (compliance) under fatigue conditions. On the other hand,  $\beta$  phase undergoes corrsoivedissociation in the inflammatory medium surrounding the implant.  $\beta$  phase dissociation reduces the durability of the implant and implies health complexity and costing surgical interventions. In this project we investigate relationships between biological corrosive environment, the mechanical load and the initial microstructure of the Ti6Al4V allov. We adopt a model-based approach interacting with other consortium partners activities (additive manufacturing, corrosion experiment, and mechanical fatigue test). to predict the evolution of beta-disscoiated phase driven by an electrochemical process in the corrosive inflammatory medium of the human body.

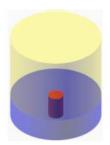


Fig. 1: Schematic of titanium alloy (Ti6Al4V) phases:  $\beta$  (red),  $\alpha$  (blue) under electrolyte (yellow)

A new implementation of in-house numerical model of ADI Alternating Directional Implicte scheme is conducted at ICP demonstrating an advanced predictive capability to describe reactive transport of ionic charges inside the metallurgical structure of titanium phases.

As exemplar case shown in this report, we introduce the evolution of reactants concentration for

a disscotiation depth of  $\beta$  phase. Similar results in corrosion pit make an evident dependency between mass migration and diffusion and the conductivity of the electrolyte. Reproducing the simulation for different pit depth values provides an explanation of the impedance spectroscopic observation correlating of measured resistance in electrolyte the pit depth, and mass transport.

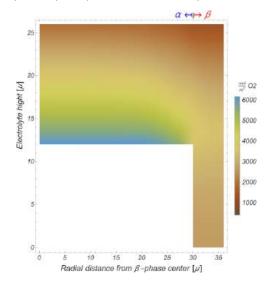


Fig. 2: Distribution of oxygen molar concentration above  $\alpha$  phase and inside  $\beta$ -dissolved pit

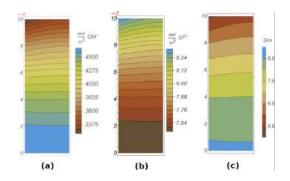


Fig. 3: (a-b) Distribution of reactants molar concentration (c) electrolyte conductivity inside  $\beta$ -dissolved pit

#### 1.6 1D model of blood vessels in arterial tree network

Worldwide, about two million patients (per year) suffering from chest pain undergo cardiac catheterization caused by Ischemia with no obstructive coronary arteries (INOCA). Using catheter-based pressure and velocity (p, v)(t) data to obtain physiological indices is the best possible way for diagnosing INOCA. At ICP we contribute a computational framework to the development of PhysioCath an innovative catheter conducted by Medyria AG. This includes flow modeling and ML. In this report we make focus on 1D model of arterial tree network.

Contributors: Y. Safa, C. Kirsch, T. Hocker Partners: USZ, EOC, Medyria AG

Funding: Innosuisse Duration: 2024–2026

PhysioCath developed by Medyria AG is an innovative catheter for diagnosing microvascular diseases by offering a unique feature for an accurate and reliable time-resolved blood pressure and velocity data. Its principle is based on obtaining the blood velocity from quantified heat source needed to maintain constant output of the temperature sensor. This sensor is combined with the heat source making an exceptional feature of PhysioCath technology. At ICP, interesting accomplishment are realized on a physical 3D thermally model to simulate the response of the PyCath sensor signals in arbitrary flow situations using inhouse code SESES and commercial CFD code. On the other hand, a 1D models of the arterial tree are considered as a good compromise between accuracy and computational cost for simulating the propagation of arterial pulse waves. Specifically, due to the simplified 1D-structural representation they are much more efficient than full 3D CFD models that intend to capture the true geometric complexity. Recall that 1D tree models with 1D governing equations of conservation of mass and momentum in combination with elastic or inelastic wall models capture many more physical details compared with 0D models.

In this project, we make use of the powerful capabilities of 1D arterial models to simulate close-to-real wave patterns. It should be realized that the information gained with PyCath yield v(t) and p(t) that are locally probed around a fixed point within the artery system, from which we then compute the corresponding wave intensities (a local time-variation of the wave power i. e. dl=dp.dv resulting as response to the heart's pumping action). Using the 1D arterial model, the local PyCath output (i.e., local v(t), p(t)) can also be simulated, and

hence, the wave analyzer can be tested with simulated data from the 1D arterial model.

A numerical challenge of modeling the 1D arterial network is to propagate waves for many periods without cumulative errors. Therefore an adequate implementation of space-time discretisation of the hyperbolic system was conducted in-house Mathematica code. The implemented numerical model accounts for forward/backward wave propagation that are described through Reimann system. The resulting signals are traced on the outlet/inlet sides where boundary conditions are informed from the upcoming characteristics.

An exemplar visualized output is shown in the Fig.1 with two time-lapses (T1 and T2) of the response of a triple bifurcation arteries to a pressure pulse at the inlet of mother vessel. The problem is solved for vessel area and for blood velocity.

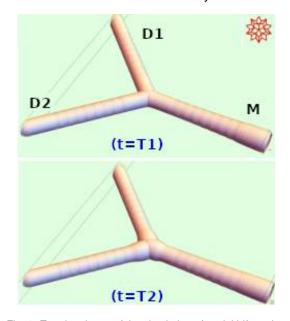


Fig. 1: Two time lapse of the simulation of artrial bifurcation including Mother (M) and two Daughters vessels (D1,2)

### 2 Electrochemical Cells

The team Electrochemical Cells and Microstructures is working on the modelling and simulation of electrochemical flow cells for various applications:

- Proton exchange membrane fuel cells are being developed to power heavy-duty vehicles like trucks. The aim is to replace combustion engines that currently run on fossil fuels. Thereby, the key technical challenge is to increase the durability of membrane electrode assemblies (MEAs).
   We are currently addressing this topic in the European project PEMTASTIC with a combination of micro- and meso-scale MEA models that allow to simulate both the cell performance and durability at power load cycling.
- Redox flow batteries (RFBs) are a technology for the grid-scale energy storage of fluctuating renewable power from photovoltaics and windmills. Aqueous organic RFBs have the advantage of low solvent cost and relatively high conductivity, and water-based electrolytes allow for safe battery operation. As a result of the European project SONAR, we have recently published a computationally efficient physics-based model of an aqueous organic RFB. The model is suitable for application in computational high-throughput screening to identify new active materials.
- Electrochemical flow cells are a key component of the future synthesis technology in the chemical industry, where electrical energy is used to power electrochemical reactions. The use of flow cells for the electro-organic synthesis will allow to produce fine chemicals or pharmaceuticals by use of renewable energy. Our team participates in the European project MiEl, where we are working on the simulation of electrode structures and the model-based analysis and design of electrochemical flow cells.



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J. Schumacher

# 2.1 Continuum scale flow cell modelling for electroorganic synthesis

MiEI is a research and training project funded by the European Union's Marie Skłodowska-Curie programme. Involving 9 partner organisations and 5 associated partners from 9 different countries, MiEI concerns the development of new synthesis technologies for the chemical industries, combining the novel advantages of electrochemistry, microprocess engineering and flow chemistry to this effect. Through the joint effort of an international network of 12 doctoral candidates, the ambitious research objective is to upscale these flow cell technologies and assemble them in arrays for the safe, flexible and sustainable synthesis of chemical products for the future, namely in the pharmaceutical industry.

Contributors: L. Vieira, J. Schumacher, R. Schärer

Partners: ICT, UvA, DTU, UWK, UCT Prague, SU, INO, ECHEM, JAN, KIT, USZ

Funding: Horizon-MSCA-2021-DN-01-01

Duration: 2023–2026

In the European doctoral network project MiEL, 12 doctoral candidates are developing electroorganic synthesis technology for the chemical industries of the 21st century, fusing the sustainable advantages of electrochemistry, microprocess engineering and flow chemistry. Electrochemical technologies have shown to offer high energy efficiency in production, while microfluidics increase safety and process control in a variety of chemical processes. As such, merging the two procedures in the form of electrochemical flow cells seems the logical step towards a more reliable and scalable, safer and greener chemical industry. The three distinct synthesis routes under investigation (twophase, aqueous and non-aqueous electrosyntheses) can be regarded as relevant model processes for this aim.

As a fundamental partner of the MiEl consortium, ZHAW-ICP's role is to enable the systematic understanding of these electrochemical processes and their feasibility by conceiving continuum scale multiphysics models of flow cells, considering the coupled effects of mass, momentum, energy, and charge transport. Via the kinetics and mass transport simulation of electrode structures subject to multi-phase fluid flow and multi-electron step reactions, the mission is to assess the performance of the developed cells by solving for current-potential distributions (Fig. 1), as well as concentration, velocity and pressure profiles.

Along with parallel work conducted by ZHAW-ICP within MiEI, different models operating on different scales will be linked, as lower scales may

provide effective parameterisations to the macrohomogenous models. Experimental model validation, parameterisation and reaction mechanism identification are all of great concern, and are being addressed for the investigated chemistries in close cooperation with the consortium. The goal of all models is to generate data reflecting material properties and to identify appropriate operating conditions of a flow cell design depending on flow rate, reactant concentrations, pressure, temperature and applied voltage, tailored to the various studied processes.

The subsequent optimization of these models (with respect to conversion efficiency, charge efficiency, and selectivity towards desired products) shall guarantee the right design and operating conditions for these technologies towards achieving the desired sustainability of industrial application, evidencing ZHAW-ICP's essential contribution to the overall project.

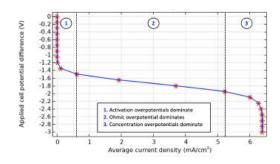


Fig. 1: Simulated polarization plot of a flow cell, breaking down the contributing influences upon the obtained cell potential difference.

#### References:

[1] MiEl project website: https://project-miel.eu/

12

# 2.2 Pore scale modeling of electrochemical synthesis processes using Lattice Boltzmann methods

Porous electrodes are central to electrochemical flow cells, an important technology crucial for electrifying the synthesis of fine chemicals. The intricate interplay of multi-phase flow, species transport, electrochemical and chemical reactions within these complex geometries presents a formidable challenge for process optimization. This research aims to develop a mesoscale Lattice Boltzmann (LB) framework to unravel these pore-scale phenomena, providing insight and generating accurate effective parameters for macrohomogeneous cell models.

Contributors: A. Dullak, R. Schärer, J. Schumacher

Partners: ICT, UvA, DTU, UWK, UCT Prague, SU, INO, ECHEM, JAN, KIT, USZ

Funding: Horizon-MSCA-2021-DN-01-01

Duration: 2023–2026

The MiEI project is concerned with the novel synthesis technologies for the chemical industry, combining the advantages of electrochemical systems, microprocess engineering, and reaction engineering. Electrochemical flow cells are essential to achieve large scale continuous production of fine chemicals. At ZHAW-ICP, our contribution lies in developing multiphysics models to deepen the understanding and optimize the performance of these critical devices. While parallel efforts focus on continuum-scale, our work is also concerned with the complex multiphysics phenomena occurring at the pore scale inside porous electrodes.

Porous electrodes are central to the efficiency and selectivity of electrochemical synthesis processes, especially in systems involving multi-phase contacting, such as reactions where gas bubbles are formed or immiscible liquid phases are involved. The intricate network of pores dictates reactant accessibility, product removal, and the overall distribution of current and potential.

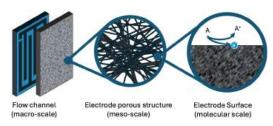


Fig. 1: Overview of the scales involved in modeling of flows in porous electrodes.

The focus of this research is the development and implementation of a Lattice Boltzmann (LB) framework to simulate two phase flows, species transport including migration and multi-step electrochemical and homogeneous reactions in realistic porous geometries. These geometries will be obtained through X-ray  $\mu$ CT imaging of actual

porous electrodes. The model is implemented to handle high viscosity and density ratios between fluid phases, along surface tension effects and interfacial dynamics by the use of free energy multiphase models and entropic and multi-relaxation time collision operators.

Beyond the simulation of reaction and transport processes at the pore scale, we aim to use the results at the pore level to upscale the information to the continuum scale. This is achieved by extracting effective parameters such as permeability or effective diffusivity, which can then inform the macrohomogeneous models. These parameters capture the essential physics information of the porous domain efficiently for cell-scale simulations.

In the current state of the work, a coupled LB simulation of fluid flow, species transport with a finite difference solver for the electric potential was implemented, incluiding an electrochemical reaction as the species transport boundary condition. The implementation was tested in a toy model consisting of the transport of ions by advection, diffusion and migration in a channel flow. The results show the expected trends in the transport of ions of opposing charges.

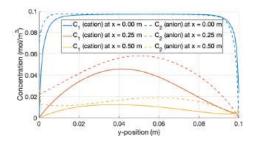


Fig. 2: Concentration profiles

Literature:

[1] MiEl project website: https://project-miel.eu/

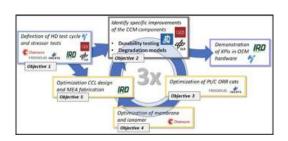
# 2.3 Robust PEMFC MEA derived from model-based understanding of durability limitations for heavy duty applications

The aim of this project is to meet the technical challenges to increase the durability of membrane-electrode assemblies (MEA) for heavy-duty vehicles applications. These challenges are approached with a combination of model-based design and development of durable catalyst coated membranes, using materials for heavy-duty operation at high temperature (up to 105°C). The target corresponds to a durability of 20'000 hours by maintaining a power density 1.2 W/cm2 at a cell voltage of 0.65V, with a platinum loading of 30g/kW.

Contributors: J.O. Schumacher, E. Scoletta, R.P. Schärer, M. Diana Partners: DLR, IRD, Imerys, CEA, Chemours, Heraeus, Symbio

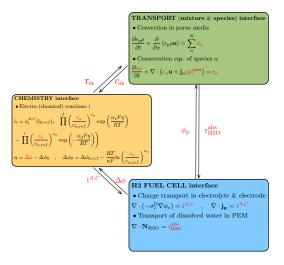
Funding: Horizon
Duration: 2023 – 2026

The project aim is to overcome the durability limitations of polymer electrolyte membrane fuel cells (PEMFCs) by developing new application-tailored component materials, cell model-based designs, and operating strategies, in line with the Strategic Research and Innovation Agenda (SRIA) of the Clean Hydrogen Joint Undertaking. The main goal is then to bring the highly innovative concept of durable heavy-duty membrane electrode assembly (MEA) to technology readiness level (TRL) 4. Different institutes contribute to this project: DLR, CEA, ZHAW are responsible for MEA characterization, ex-situ analysis and model-based designs. Component suppliers (IRD) and material suppliers (IMERYS, Heraeus, Chemours) are responsible for providing the innovated and improved different sub-components of the catalyst coated membrane (CCM).



Workflow methodology of the PEMTASTIC partners.

We have been developing a one-dimensional PEMFC model of a differential test cell accounting for the through-plane transport of gas species, water, charge, and heat, and for the electrochemical reactions in the catalyst layers. Moreover, we can simulate performance decay due to chemical membrane degradation and catalyst layer degradation.



Coupling diagram of the PEMFC differential test cell model.

Chemical membrane degradation is caused by the formation of hydroxyl radicals. These radicals are generated through reactions involving hydrogen peroxide, a common byproduct in fuel cells, under the influence of metal ions such as iron. Our model describes hydroxyl radical attack of the polymer bonds within the membrane, causing chain scission and loss of mechanical membrane integrity. Moreover, we have implemented a catalyst layer degradation model [1] and coupled it to our performance-degradation model. We can now simulate performance decay due to decrease of membrane protonic conductivity and platinum particle growth leading to loss of electrochemical surface area in the catalyst layers. Additional work is planned to integrate effective properties obtained from meso-scale modeling and modelorder-reduction to reproduce the fuel cell dynamics during vehicle driving cycles.

#### Literature:

[1] A. Kregar et al., *J. Power Sources*, Vol. 514, 230542, 2021.

### 2.4 Mesoscale Modelling of the Catalyst Layer in PEMFCs

Proton exchange membrane fuel cells (PEMFCs) are a promising technology contributing to the decarbonization of the industry and transport sector. The European-funded PEMTAS-TIC project aims to increase the durability of membrane electrode assemblies (MEAs) for PEMFCs by a combined experimental and modelling approach. The cathode catalyst layer strongly impacts the overall performance due to the sluggish oxygen reduction reaction. Furthermore, the longevity of the fuel cell is affected by critical degradation phenomena, such as carbon corrosion, platinum dissolution, or ionomer degradation. At ICP, we are developing mesoscopic models with the aim of better understanding the coupled processes at the mesoscale and developing improved parameterisations for macrohomogeneous cell models.

Contributors: R. P. Schärer, E. Scoletta, M. Diana, J. O. Schumacher Partners: DLR, IRD, Imerys, CEA, Chemours, Heraeus, Symbio

Funding: Horizon
Duration: 2023 – 2026

In PEMFCs, the cathode catalyst layer provides the reactive sites for the oxygen reduction reaction. This layer is composed of carbon particles providing the overall structural support, catalytic platinum nanoparticles, and proton-conducting ionomer. While the overall oxygen reduction reaction is often simplified as  $4\mathrm{H}^+ + 4\mathrm{e}^- + \mathrm{O}_2 \to 2\mathrm{H}_2\mathrm{O}$ , the actual process proceeds through complex multi-step reaction pathways involving multiple intermediate species and competing reactions.

The oxygen reduction reaction (ORR) on platinum surfaces involves sequential electron transfer steps that can lead to different reaction products depending on the local electrochemical environment. A critical aspect is the formation of hydrogen peroxide as an intermediate species, which not only affects the overall reaction efficiency but also serves as a key reactant in membrane degradation processes. Additionally, the platinum surface undergoes dynamic changes through the formation of oxide layers, which significantly influence the local chemical environment at the reaction plane within the double layer structure.

Understanding these coupled multi-step surface reactions is crucial because intermediate species can block available active surface sites, reducing catalytic activity. Furthermore, the interconnected nature of these reactions drives parasitic processes such as carbon corrosion, where the weakened structural integrity of the carbon support can ultimately lead to microstructure collapse and significantly altered transport resistances.

At ICP, we develop transient and spatially-resolved models that explicitly capture these multi-step reaction pathways through a unified framework coupling the ORR, hydrogen peroxide formation, and carbon corrosion reactions as shown in Figure 1. Our approach integrates a double layer model that accounts for oxide layer formation on the platinum surface, enabling accurate prediction of the local chemical environment at the reaction plane.

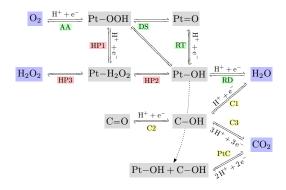


Fig. 1: Heterogeneous multi-step reactions on the platinum and carbon surfaces.

The multi-step surface reaction model is coupled to mass transport equations for mobile species. To capture the local transport resistances, we consider the diffusive transport through the porephase, water layers, and ionomer thin films over the reactive Pt nanoparticles. Additionally, we consider the dynamic evolution of the two-phase liquid-gas mixture in the porous catalyst structure, which critically affects local transport resistances and influences the concentration of reactive species at catalytic sites.

#### Literature:

[1] PEMTASTIC project web site: https://pemtastic-project.eu/

### 2.5 Multi-scale Modelling of Organic Redox Flow Batteries

Redox flow batteries (RFBs) are a promising technology for the stationary energy storage from renewable energy sources. Organic molecules are an attractive alternative to conventional metal-based electrolytes because they can be synthesised locally, thus reducing supply chain risks. Within the European Marie Skłodowska-Curie Doctoral Network PRE-DICTOR, a rapid, high-throughput method is being developed to identify and develop materials for electrochemical energy storage. This revolutionary approach comprises modelling and simulation tools for computational screening of organic chemicals, automated chemical synthesis and characterisation, artificial intelligence-based self-optimisation methods, and data management systems.

Contributors: R. P. Schärer, J. O. Schumacher

Partners: ICT, SCAI, DTU, CNRS, KIT, UNSW, Aalto University, CEB, CellCube, SCM, AM

Funding: European Union's Marie Skłodowska-Curie programme

Duration: 2024–2028

RFBs represent a promising electrochemical energy storage technology where energy is stored in liquid electrolytes containing dissolved electroactive molecules. These electrolytes are circulated through electrochemical flow cells, where the molecules undergo reversible redox reactions at electrode surfaces, enabling energy storage and release through electron transfer in the two halfcells. This architecture allows independent scaling of power and energy capacity, making flow batteries attractive for grid-scale applications requiring long-duration storage.

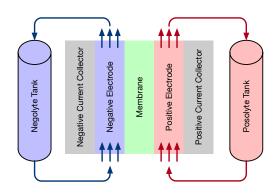


Fig. 1: Simplified geometry of a flow battery cell.

Within the PREDICTOR project [1], high-throughput methods are being developed that will revolutionize the screening and development of materials for electrochemical energy storage. The project focuses on redox flow batteries as one of the most promising technologies for medium- to long-term energy storage, where the accelerated development of organic electrolytes offers signifi-

cant potential to improve these systems and tailor them for specific applications.

The project encompasses three areas: 1) modelling, simulation and computational screening, 2) experimental high-throughput methods, and 3) data management and validation. An existing computational screening method based on a digital battery twin from the EU-funded SONAR project serves as the starting point for screening conventional and shuttle-based RFBs.

Fig. 2: Multiscale modelling approach of porous electrodes.

Homogenization Thin double layer approximation

ICP contributes to the PREDICTOR project by supervising two PhD candidates working on critical modelling components. The first PhD project focuses on processes at the electrochemical interface by describing the double layer structure and multi-step reactions. This interfacial model will be integrated into pore-scale models to describe reactive mass transport in porous electrodes and derive macroscopic transport properties (see Figure 2). The second PhD project develops macroscopic cell-scale models (see Figure 1) to describe the coupled transport of mass, charge, and energy. This work focuses on developing and integrating thermodynamically consistent membrane models. Additionally, ICP actively contributes to data management, which is critical for the project's success.

Literature:

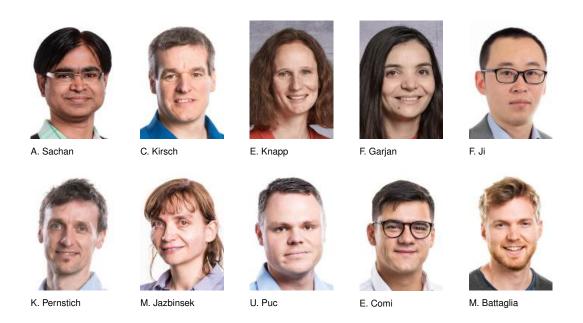
[1] PREDICTOR project web site: https://www.rfb-predictor.eu

## 3 Organic Electronics and Photovoltaics

Organic semiconductors are used in a wide range of applications mostly in the form of OLED displays in everyday products that are used by mobile phones up to 77-inch TVs.

The particular advantages of OLEDs are their thin construction, large viewing angle, color gamut and high energy conversion efficiency. OLEDs consist of a sequence of thin organic semiconductor layers placed in-between two metallic electrodes. Organic semiconductors have equally gained attention as strong light absorber and charge transport materials in organic solar cells, with which flexible PV modules can be built. In recent years, organic semiconductors have also been key to the ground-breaking hybrid organic-inorganic perovskite solar cell technology, which is the hottest emerging photovoltaics technology and shows great potential for LED and memristor applications, too. Luminescent quantum dots are important ingredients in novel displays and thus are also subject of our research. Further into the invisible range of electromagnetic waves, terahertz photonics is a growing technological field for non-invasive diagnostics applications.

The ICP carries out R&D in the field of OLED, OPV, perovskite PV and non-linear optical crystals for terahertz photonics technology by employing multi-physics computer models and devising novel measurement systems. In the laboratory of the ICP, we fabricate OLEDs and novel solar cells on a small scale for R&D purposes and have set up a novel terahertz photonics measurement system for diagnostic purposes. We focus on device and material characterization methods by a combination of advanced measurement and simulation technology and have gained experience with machine learning. This chapter gives an overview on ongoing R&D projects carried out in this interdisciplinary research field of the ICP.





M. Auer



M. Torre



O. Zbinden



B. Ruhstaller



W. Tres



R. Wirth



T. Krucker



T. Sachsenweger

# 3.1 Terahertz imaging of encapsulation films for Perovskite solar cells

Within the scope of the Innosuisse-KIAT international research project *PACSTATE*, one of the goals is to develop terahertz imaging and characterization methods for novel encapsulation films used in perovskite solar cells. By utilizing terahertz technology, we aim to gain a better understanding of the underlying physics and long-term stability of the encapsulation materials, thereby enhancing the performance and lifespan of the perovskite solar cells.

Contributors: U. Puc, M. Auer, M. Jazbinsek

Partners: Solaronix, Fluxim, ZHAW-IMPE, Ajou University, UNIS, Pusan National University

Funding: Innosuisse – KIAT South Korea

Duration: 2024–2026

The terahertz (THz) system developed at ZHAW ICP is used to investigate the encapsulation materials for perovskite solar cells in this project. The aim is to utilize THz technology for advanced non-destructive testing (NDT) methods to evaluate the uniformity of the new materials, degradation by-products, and optical/electrical properties that affect the final photovoltaic performance. Our THz system is based on organic electro-optic crystals and can generate and detect ultra-broadband THz waves with a frequency range of up to 20 THz.[1] This provides us with a unique advantage over other commercially available THz systems in detecting far-infrared molecular vibrations and phonon modes (optical lattice vibrations) in various materials, as well as charge transport phenomena in conducting or semiconducting materials, [2,3].

Encapsulation films are commonly used to extend and preserve the performance of solar cells by limiting the ingress of environmental factors such as humidity and oxygen. However, these encapsulants must be optimized to achieve maximum performance when applied to perovskite solar cells. To accomplish this, we are investigating various types of novel encapsulants using THz waves by examining material modifications after they are applied to perovskite cells. Moreover, we are examining the homogeneity of the films by analyzing thickness uniformity and defects. THz imaging is an ideal tool for such investigations, as it is extremely sensitive to variations in thickness and defects on

the surface or within the material. An example of THz imaging of encapsulation materials with multiple surface defects is shown in the image.

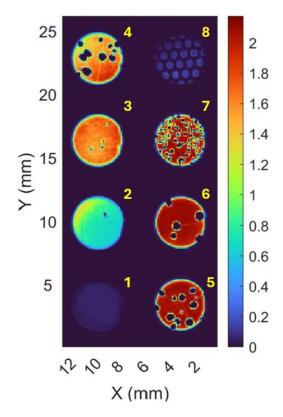


Fig. 1: THz amplitude imaging of encapsulant materials revealed surface defects that developed after the material was subjected to various temperatures. The temperatures investigated were as follows:  $1-80\,^{\circ}\text{C},\,2-90\,^{\circ}\text{C},\,3-110\,^{\circ}\text{C},\,4-130\,^{\circ}\text{C},\,5-150\,^{\circ}\text{C},\,6-170\,^{\circ}\text{C},\,\text{and}\,7-200\,^{\circ}\text{C}.$  The original material (Nr. 8) was assessed at room temperature. The resolution of the THz imaging was 100  $\mu\text{m}$ .

#### Literature:

[1] Puc, Bach, Günter, Zgonik, Jazbinsek; Adv. Photonics Res. 2 (2021). https://doi.org/10.1002/adpr.202000098

[2] Puc, Yang, Kim, Kwon, Jazbinsek; Opt. Mater. Express 13 (2023). https://doi.org/10.1364/OME.475427

[3] Santhosh, Puc, Jazbinsek, Oberlintner, Shvalya, Zavasnik, Cvelbar; Appl. Surf. Sci. 682, 161698 (2025). https://doi.org/10.1016/j.apsusc.2024.161698

### 3.2 Terahertz spectroscopy of complex chalcogenides

In this Swiss-Ukrainian joint research project, we aim to explore the ultra-broadband terahertz (THz) properties and functionalities of chalcogenide crystals. By obtaining new valuable information about (photo)conducting, dielectric and nonlinear optical parameters of these materials, we aim to identify new materials for generation, modulation and detection of THz radiation. The ICP is responsible for the optical, nonliner optical and THz characterisation of the crystals, which are prepared by the Ukrainian partner.

Contributors: M. Auer, U. Puc, M. Jazbinsek

Partners: Uzhhorod National University (Ukraine)

Funding: SNSF Duration: 2025–2028

For THz photonics, the measurable spectrum is strongly depending on the used THz source and detector material. Highly nonlinear optical molecular crystals offer unique advantages for THz-wave generation compared to alternative methods. They have a much broader THz generation range, which can cover the whole THz range from 0.1-20 THz. However, the most organic crystals lead to undesired modulation of the spectrum and limited output efficiency due to phonon-induced absorption [1-3]. At ICP, we use organic crystals as THz source and detector, which leads to a measurable THz range around 20 THz [4]. THz timedomain spectroscopy (THz-TDS) experiments can

be performed in a transmission or a reflection setup. Transmission setups give more accurate results and are easier to implement and are therefore mostly used. However, the measurable absorbance is limited and strongly absorbing samples can only be measured in a reflection setup. The setup at ICP is designed in a way, that it can be switched from transmission to reflection geometry. With both measurement geometries available and a broad THz range the THz system at ICP is optimal to extract the THz properties of complex samples like chalcogenides and to identify possible materials for THz photonic applications.

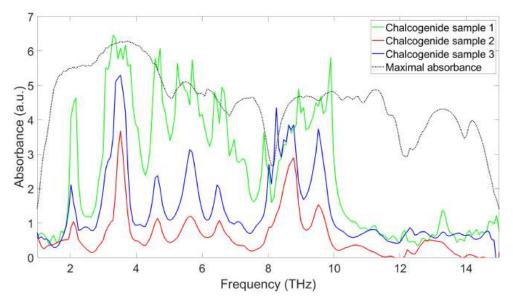


Fig. 1: The measured absorbance of three chalcogenide single crystals with different thicknesses using THz-TDS in transmission mode at ICP. The peaks indicate many phonon modes, which are responsible for the dispersion of the dielectric susceptibility [4]. The dotted line indicates the maximum measurable absorbance in transmission, which is reached for several peaks for the thickest sample (sample 1) in this example.

- [1] Kwon, O-Pil and Jazbinsek, Mojca, J. Mater. Chem. C Vol. 12, No. 35, 2024.
- [2] Park, Kim, Auer, Shin, Yoon, Yun, Yu, Puc, Kim, Jazbinsek, Rotermund, Kwon, *Applied Physics Reviews Vol. 12, No. 1*, 2025.
- [3] Lee, Puc, Kim, Jazbinsek, Kwon, Advanced Optical Materials Vol. 12 No. 13, 2024.
- [4] Puc, Bach, Günter, Zgonik, Jazbinsek, Adv. Photonics Res. 2 2021.

# 3.3 Design and Development of Industry Compatible Characterisation Equipment for Emerging Perovskite and Perovskite/Silicon Tandem Solar Cells (DICE)

This Swiss/Finnish innovation project aims to develop innovative testing systems for emerging solar technologies, with a focus on perovskite and perovskite/silicon tandem cells. Central to DICE are an industrial high-speed solar simulator, a multispectral imaging tool for quality control, and simulation models to investigate ion migration and its impact on device performance.

Contributors: E. Comi, C. Kirsch, E. Knapp

Partners: Endeas Oy, Fluxim AG, Abo Akademi, Tampere University, EPFL

Funding: Eureka/Innosuisse

Duration: 2024-2027

Perovskite solar cells (PSCs) and perovskite/silicon tandem solar cells (PSTs) are among the most promising approaches for highefficiency photovoltaics. While PSCs have already achieved certified power conversion efficiencies (PCEs) of 26.1%, PSTs have reached nearly 35%. By combining the advantages of both technologies, there is significant potential for industrial application.

A key characteristic of PSCs is the presence of mobile ions, which influence transient processes. These affect the electrical response of the cells and lead to phenomena such as hysteresis and scan-rate dependence in IV measurements. This presents a challenge for fast and accurate efficiency determination, which is essential for industrial production processes.

The Finnish industry partner Endeas has extensive experience in inline measurement of silicon cells and can record IV characteristics within seconds. The goal is to adapt this measurement technology for PSTs. However, due to the complex transient behavior of PSCs, additional data interpretation is required. This is where simulations become advantageous.

ICP and Fluxim use the software Setfos, which is based on drift-diffusion models and can simulate time-dependent ion migration processes in solar cells. A precise model can help to assess the steady-state performance of PSTs through parameter extraction and machine learning.

A further challenge for the industrization is the upscaling of PSTs that often leads to lateral inhomogeneities and defects. These can be analyzed using imaging techniques such as photolumines-

cence (PL), electroluminescence (EL), or lock-in thermography (DLIT, ILIT). Fluxim and the ICP have already developed a multispectral imaging system (see Fig. 1), which will now be expanded for PST characterization, especially in terms of a camera and an illumination source that cover the necessary spectral range. Additionally, the 1D+2D simulation tool Laoss will be extended with a third electrode to enable realistic simulation of lateral effects in tandem cells.



Fig. 1: This imaging prototype is being further developed in the DICE project.

#### 3.4 Investigating charge transport in organic semiconductors with electrochemical methods and modelling

Today organic semiconductors are used in many technological applications. However, these materials must be thoroughly studied in order to design even better products. Our project aims to improve the characterization of organic semiconductors using electrochemical measurements in combination with computer simulations.

Contributors: Ş. C. Cevher, G. Kissling, B. Ruhstaller, K. P. Pernstich

Partners:

SNSF Funding: **Duration:** 2020-2025

Nowadays organic semiconductors are widely used in display and lighting applications and in the fabrication of novel transistors, sensors and solar cells. In order to produce better devices, the understanding of the physical processes and the materials properties of organic semiconductors needs to be improved. In this interdisciplinary project we investigate organic semiconductor materials using electrochemical methods and multiphysics modelling.

The aim of the project is the development of a reliable method for the characterization of a range of organic semiconductor properties and materials parameters. The experiments will give us insight into some properties which have so far been very hard or almost impossible to measure.

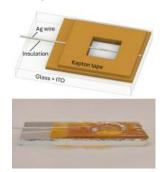
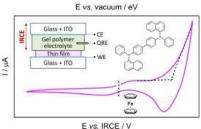


Fig. 1: Integrated Reference-Counter Electrode (IRCE) with Kapton tape securing the partially insulated Ag wire and creating a reservoir for the gel polymer electrolyte.

We initially used electrochemical methods in solution to characterize the energy levels of organic semiconductor molecules [1]. While this approach is straightforward, it has a major drawback: the measured energy levels often differ from those in the solid state, where these materials are actually used. To overcome this limitation, we developed and recently published a novel technique [2] that enables electrochemical measurements directly on thin films. At the heart of this method is an integrated reference-counter electrode (IRCE), which is shown in Figure 1. It consists of a small reservoir of gel polymer electrolyte and an embedded silver wire acting as a quasi-reference. The compact structure can be gently pressed onto a semiconductor-coated substrate, allowing voltammetry to be performed on thin films.

This setup was used, for example, to measure a thin film of the OLED material NPB. To calibrate the measurements, we coated the IRCE with a thin layer of ferrocene, a well-known redox standard. The resulting voltammogram shown in Fig. 2 clearly displays both the ferrocene peaks and the onset of NPB oxidation. From this data, we extracted the HOMO energy of NPB to be -5.43 eV, which matches well with literature values obtained by more complex methods. This confirms that our technique can provide reliable and accessible energy level measurements in actual device-like conditions. We believe this method has the potential to become a standard tool for organic electronics research.



E vs. IRCE / V

Fig. 2: Electrochemical measurement of an NPB thin film using the integrated reference-counter electrode (IRCE). The voltammogram shows both the ferrocene redox peaks (used for calibration) and the onset of NPB oxidation, from which the HOMO level is determined. This demonstrates that the IRCE enables reliable energy level measurements directly in thin films.

[1] G. P. Kissling et. al., doi: 10.1016/j.orgel.2023.106888 [2] S. C. Cevher et al., doi: 10.1016/j.orgel.2024.107152.

### 3.5 Accelerated aging and modeling of perovskite solar cells

As part of this SNSF-funded research project in collaboration with the Saule Research Institute in Poland, we aim to rapidly and reliably understand, model, and predict the degradation of perovskite solar cells through accelerated aging combined with non-destructive in-situ characterization. To support this, we have developed a custom in-house aging setup capable of varying light intensity and temperature, while maintaining the device at maximum power point or other critical operating conditions.

Contributors: S. P. Shaji, K. Meraji, W. Tress

Partners: Saule Research Institute Wroclaw Poland

Funding: SNSF Duration: 2023–2027

Perovskite solar cells (PSCs) represent one of the most rapidly advancing photovoltaic technologies, having achieved unprecedented gains in power conversion efficiency (PCE) compared to other solar cell types. Despite laboratory-reported efficiencies exceeding 26.9% after nearly two decades of research, their widespread commercialization remains hindered by a critical challenge: long-term operational stability.

Accelerated aging techniques enable rapid and accurate assessment of device lifetimes under realistic operating conditions [1]. This project seeks to tackle the stability issue by employing controlled stress factors to induce degradation, while utilizing in situ characterization methods to probe underlying degradation mechanisms under realworld conditions. To analyze the resulting high-dimensional data, we integrate big data analytics. We have developed a custom-built accelerated aging platform that allows precise tuning of illumination intensity from 0.1 to 10 suns and temperature control from 10°C to 100°C. The setup is

designed to be modular and glovebox-compatible, enabling degradation studies in various controlled atmospheres. In parallel, we are developing machine learning algorithms capable of analyzing the rich datasets produced via in-situ measurements during stress testing, with the goal of extracting rapid insights into evolving charge transport and degradation signatures.

In the long term, this research aims to significantly accelerate the development of stable perovskite photovoltaics, facilitating their integration into the global energy market. Such progress would contribute meaningfully to decarbonization efforts and mitigate the impacts of climate change on our society.

#### Literature:

[1] Zhao, X., Liu, T., Burlingame, Q.C., Liu, T., Holley III, R., Cheng, G., Yao, N., Gao, F., Loo, Y.L., Accelerated aging of all-inorganic, interface-stabilized perovskite solar cells. Science, 377(6603), pp.307-310, 2022.

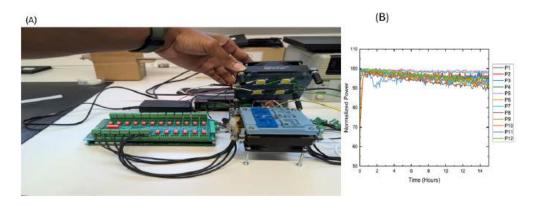


Fig. 1: (A) Aging setup with 24 channel MPP board and temeperature and light intensity controlled stage (B) Stability data of some perovskite cells which were fabricated in our lab.

# 3.6 Autoencoder for Parameter Estimation and Device Simulation of Perovskite Solar Cells

Knowing the physical processes is important for a deep understanding of perovskite solar cells (PSCs). For this, it is important to know the behavior of charge transport or recombination, for example. However, some key parameters related to these processes cannot be measured directly or only with great effort and high uncertainty. To tackle these issues, an approach that uses a combination of device simulation and Machine Learning (ML) is used. Applying the method to real-world devices shows the practical relevance of this study.

Contributors: O. Zbinden, E. Comi, E. Knapp, W. Tress

Partners:

Funding: ERC Duration: 2023–2025

Within only a decade, the power conversion efficiency of PSCs has dramatically increased, reaching almost 27%. However, PSCs are still not fully understood. To push the technology of PSCs to the next level, it is crucial to gain a deeper understanding of these devices.

Here, a PSC device is simulated with a driftdiffusion model. This initial device is then used as a starting point to vary parameters of interest in a random combination, all of them within physically reasonable boundaries. The dataset generated in this way can then be used to train an ML model. Fig. 1 shows the used model, an Autoencoder (AE) which is modified by a custom loss function that not only acts on the output, but also on the latent parameter space. The encoder takes an ndimensional input, the current, and transforms it to the so-called latent space with a chosen dimensionality m, in this case corresponding to the randomly varied parameters in simulation. The decoder then takes these latent parameters and tries to reconstruct the n-dimensional input data.

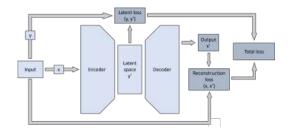
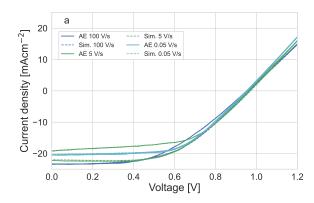


Fig. 1: The currents, denoted as x, are passed to the encoder part of the AE. The true parameter values y, known from simulation, are not passed to the encoder, they only act on the loss function.

After the AE is trained, the encoder and decoder can be used independently. The encoder is used to predict physical parameters, and the decoder mimics a fast device simulator. To demonstrate the reliability of the AE predictions, the estimated parameters are again used in simulation, and the results are compared to the experimental measurements. Additionally, these simulations are compared to the current-voltage (J-V) curves predicted by the AE, to show how well ML performs on this task.



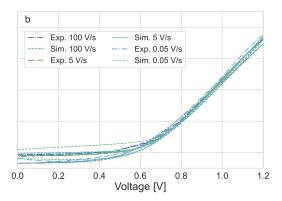


Fig. 2: a compares the J-V curves predicted by the decoder and the simulation based on the estimated parameters. The results are almost identical, the decoder is 1000 times faster than the device simulation to obtain these curves. b: Measured J-V curves and the simulation, based on the AE-estimated parameters. The overall shape is covered very well, but some details are missed due to limitations in simulation.

### 3.7 Ion Migration in Perovskite Solar Cells

In this project we are investigating how mixed ionic-electronic conductivity affects the performance of perovskite solar cells. Depending on their distribution in perovskite, mobile ionic charges can modify the ability of the solar cell to extract current under illumination. We are developing new characterisation approaches based on spectrally resolved measurements with temperature control, which can help to elucidate the device physics of perovskite solar cells.

Contributors: M.A. Torre, W. Tress

Partners:

Funding: ERC

Duration: 2021–2025

Mobile ionic charges in perovskite solar cells (PSCs) can screen the electric field, reducing the driving force for charge extraction. We recently showed that ionic field screening can be visualised as spectral changes in the External Quantum Efficiency (EQE) [1], as seen in Fig. 1a. For carbon-based PSCs, the EQE drops at longer wavelengths with ionic screening, indicating that current losses mainly originate from charges generated deeper in the absorber. We can compare the effect of different ionic distributions on the EQE by cooling the device under different voltages, effectively freezing the ions.

The slow response of mobile ions to changes in the applied voltage leads to scan rate-dependent hysteresis in the current density-voltage (J-V) curve [2], as shown in Fig. 1b, where a significant cur-

rent loss ('bump') appears in the backward (BW) scan. By controlling the temperature, setting the initial precondition, and varying the bias voltage for EQE measurements in the same order as in the J-V scan, we can reconstruct the J-V curve with spectral information, enabling direct visualisation of ionic screening and the origin of hysteresis (Fig. 1c). Varying the temperature such that ions can respond during the voltage scan mimics the effect of changing the scan rate, as ionic mobility is strongly temperature-dependent. This approach allows us to explain current losses and J-V hysteresis from inferred changes in the spatial collection efficiency caused by mobile ions. We are applying this characterisation method to different PSC architectures and complement it with optical and drift-diffusion simulations to deepen our understanding of PSC device physics.

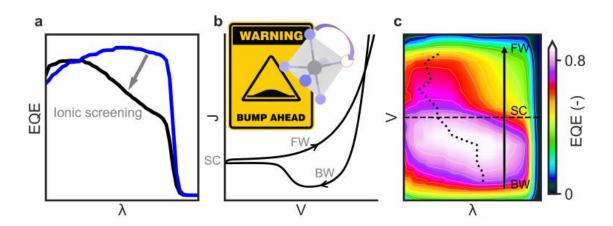


Fig. 1: a) EQE of a carbon-based PSC measured at low temperature, comparing the effect of different ionic distributions (cooling voltages). b) J-V curve, showing hysteresis and a current loss before short-circuit (bump). c) EQE-V map for the J-V curve in b).

#### Literature:

[1] M. A. Torre Cachafeiro, E. L. Comi, S. Parayil Shaji, S. Narbey, S. Jenatsch, E. Knapp, W. Tress, *Adv. Energy Mater.*, 15, 2403850, 2024.

[2] W. Tress, N. Marinova, T. Moehl, S. M. Zakeeruddin, M. K. Nazeeruddin, M. Grätzel, *Energy Environ. Sci.*, 8, 995–1004, 2015.

### 3.8 Down-conversion White Light-Emitting Diodes Based on Lead-free Perovskite Derivatives

The development of efficient and eco-friendly white Light-Emitting Diodes (LED) materials is crucial for advancing next-generation lighting technologies and achieving carbon neutrality goals. Here, we have developed a series of novel, stable, and non-toxic lead-free perovskite derivatives that exhibit diverse emission colors, some of which can be successfully applied in down-conversion white LED.

Contributors: F. Ji. W. Tress

Partners:

Funding: SNSF (Postdoctoral Fellowships)

Duration: 2023–2025

With the growing demand for sustainable and lowpower lighting, white LEDs have become a major focus in materials science. Designing new luminescent materials is essential to improve performance while eliminating toxic or unstable components

Metal halide perovskites have attracted substantial attention as potential luminescent materials for LEDs, owing to their tunable bandgaps, high photoluminescence quantum yields, and solution-processability. Despite these advantages, dominant lead-based perovskites exhibit narrow emission spectra due to band-to-band radiative recombination, necessitating the combination of multiple emitters (red, green, and blue) to generate white light. Furthermore, the inherent toxicity of lead and the limited stability of these materials severely constrain their practical applications in lighting technologies.

To overcome these limitations, we developed a series of bismuth and antimony-based lead-free perovskite derivatives, which are non-toxic and exhibit significantly improved environmental stability. These materials exhibit self-trapped exciton (STE) emission, a unique exciton recombination process that typically results in broadband photo-

luminescence and is highly desirable for achieving single-component white-light emission. As illustrated in Figure 1a, we prepared a series of compounds with a general formula  $A_x BX_{(3+2x)}$ , where A is organic cations and X is halide anions. Here, we mainly take three representative materials—S-1 to S-3—as examples to demonstrate that their emission properties can be systematically tuned by compositional modification, exhibiting diverse photoluminescence under ultraviolet excitation, including blue (S-1), warm yellow (S-2), and red (S-3).

Among them, the S-2 sample emits a warm, yellow light under excitation by a 254 nm UV lamp, which closely resembles white light. We therefore coated S-2 onto a 275 nm commercial LED chip to fabricate a down-conversion white LED device. As shown in Figure 1b, the resulting LED emits white light, attributed to the STE emission from S-2. The luminescence intensity increases with increasing input current (Figure 1c), confirming the material's excellent down-conversion capability and potential for solid-state lighting applications. These materials would hold even greater application potential if they could be further developed for use directly in electroluminescent white light LED devices in the future.

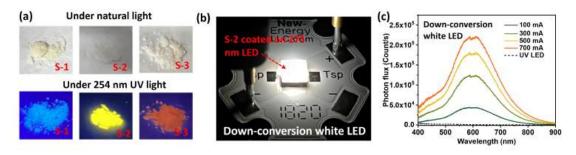


Fig. 1: a) Optical images of three lead-free perovskite derivatives under natural light and 254 nm UV light. b) Down conversion white LED based on S-2 material coated on a 275 nm LED. C) Current-dependent emission of the down-conversion white LED.

# 3.9 Understanding and Manipulating Resistive Switching in High-Performance Memristors

We study the device physics of emerging perovskite semiconductors—both in solar cells and memristors—by fabricating and characterizing a wide range of memristor stacks. Our goal is to uncover the origin of their ultra-fast resistive switching, in which a ten-orders-of-magnitude  $(\approx 10^{10})$  current jump occurs in just tens of nanoseconds. Understanding this abrupt transition is key, since it's precisely that speed-and-contrast combination that makes memristors attractive. Beyond high-density, non-volatile memory, these devices are being pursued as artificial synapses for neuromorphic hardware and as low-power, in-memory Al accelerators.

Contributors: M. Mohammadi, W. Tress

Partners:

Funding: ERC Duration: 2021–2025

Solar cells based on metal-halide perovskite absorbers became the rising star in photovoltaics research. Their outstanding opto-electronic properties enabled a power-conversion efficiency exceeding 26%. While developing these devices, researchers observed a pronounced hysteresis in the current–voltage (I-V) curve. Follow-up studies revealed a slow transient response and a strong dependence on the voltage-sweep rate, providing compelling evidence that mobile-ion migration is responsible for the hysteresis.

Although hysteresis is usually considered a drawback in perovskite solar cells, the same behaviour is a virtue in resistive-switching devices such as memristors. The looped (I-V) response naturally furnishes two stable, non-volatile resistance states that can be toggled with moderate forward and reverse voltages (1 V). After programming, the state is checked with a small read voltage; under this gentle bias the response is nearly ohmic, revealing either a low-resistance  $\bf ON$  state or a high-resistance  $\bf OFF$  state.

Most memristor stacks still require an initial formation (or electroforming) step in which voltages above 2 V are applied before reliable programming is possible. This high-voltage conditioning raises power consumption, introduces device-to-device variability, and can accelerate dielectric degradation—factors that hinder large-scale integration. In our recent work we engineered a memristor that operates without any forming step, yet retains benchmark performance. This forming-free architecture removes a major bottleneck for deploying memristors in neuromorphic and non-volatile memory hardware.

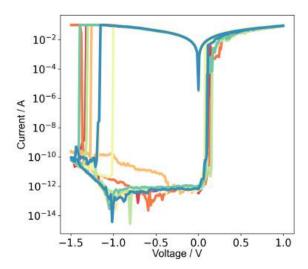


Fig. 1: I-V curves of a memristor after formation

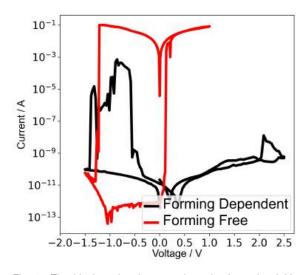


Fig. 2: The black and red traces show the formation I–V curves for a forming-dependent and a forming-free memristor, respectively. Compared to Fig. 1, the formation trace of the forming-free memristor is identical to its post-formation I–V curves.

### 3.10 Characterization and Modelling of Interfaces in Perovskite-Silicon Tandem Devices

Our work focuses on understanding and controlling interface-related losses in emerging tandem solar cell technologies that combine metal-halide perovskites with silicon. These tandem devices offer the most promising route to push photovoltaic efficiencies beyond the single-junction limit of silicon. However, scaling such devices from small lab samples to industrially relevant modules introduces new challenges related to interfacial recombination, charge extraction, and mechanical stability—many of which are not well understood at the microscopic level.

Contributors: K. Meraji, T. Krucker, B. Ruhstaller, W. Tress

Partners: EPFL (PV-LAB), CSEM (PMD,NANO), FLUXIM, KTU

Funding: SNSF (Sinergia)
Duration: 2024–2028

Our group leads a multiscale characterization and modelling platform to probe the functional properties of self-assembled monolayers (SAMs) at the nanometre scale. We combine electro-optical measurements with numerical simulations using drift-diffusion models that account for mobile ions and photon recycling. These studies reveal how SAMs modify charge transport, energy barriers, and recombination at buried interfaces.

At the device level, we evaluate the electrical and optical behavior of single-junction and tandem cells using steady-state and transient methods. This helps identify loss mechanisms and informs

material selection and processing strategies. We also study the upscaling process from lab-scale devices to mini-modules, with a focus on how spatial inhomogeneities and interconnects affect performance. For example, EL characterization will be performed on the submicron scale using confocal microscopy to elucidate the effect of SAMs on the emission and visualize how the conformity of perovskite films over microtextured silicon substrates affects device stability Figure 1. Combining characterization and simulation, we aim to correlate fabrication quality with long-term stability under operational conditions.

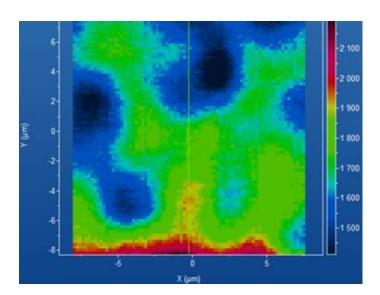


Fig. 1: Electroluminescence mapping of a silicon-perovskite interface revealing spatial variations in emission intensity.

# 3.11 Understanding Solar Cells at Nanoscale for Efficient Renewable Energy

Perovskite solar cells (PSCs) have achieved remarkable efficiency gains, yet further improvements demand insights into nanoscale phenomena affecting performance. This project explores the structural and optoelectronic properties of PSCs using atomic force microscopy (AFM) and complementary spectroscopy. By analyzing grain boundaries, defects, and interfaces, we aim to uncover mechanisms that limit efficiency and stability, guiding the development of more efficient and durable solar cells.

Contributors: A. K. Sachan, L. N. Schusser, T. Sachsenweger Ballantyne, F. Ji, W. Tress

Partners:

Funding: ERC Starting Grant

Duration: 2020-2025

Photovoltaics (PV) are central to a sustainable, low- $CO_2$  energy future. PSCs have seen a rapid rise in power conversion efficiency (PCE) from  $\sim\!3\%$  to over 25% in just a decade. However, further progress toward the theoretical limit ( $\sim\!33\%$ ) requires a better understanding of nanoscale structures within the perovskite layer, which consists of polycrystalline grains (10–500 nm) separated by grain boundaries (GBs). Imperfections and defects at GBs and within grains introduce trap states that hinder device performance.

We use advanced AFM techniques—such as Kelvin probe force microscopy (KPFM) and conductive AFM (cAFM)—to map surface potential, conductivity, and work function at the nanoscale. These methods reveal how grain structure, defects, and interfaces affect charge carrier behavior. A novel cross-sectioning approach enables direct access to buried interfaces, allowing us to probe structural and functional changes under electrical bias, light exposure, and varying environments.

To achieve a comprehensive picture, we combine AFM-based techniques with Raman and photoluminescence spectroscopy in colocalized studies. This multi-modal approach provides insights into both morphology and optoelectronic behavior, in-

forming the design of PSCs with enhanced efficiency and long-term stability. Our findings will also contribute to broader materials science applications in nanotechnology and energy systems.

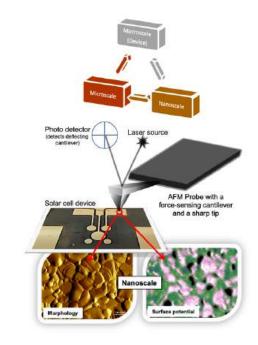


Fig. 1: High-resolution investigation of solar cell properties using atomic force microscopy and Kelvin probe force microscopy.

## 4 Sensor and Measuring Systems

Our team of talented ZHAW engineers and scientists has been applying for more than ten years well established and emerging measurement methods to relevant medical and biological problems. We collaborate with startups, international companies as well as leading academic partners and bring our engineering expertise to projects requiring state-of-the-art technical development.

We have been dedicated to creating impact by cultivating an entrepreneurial mindset and thinking beyond academic publishing, focusing on technology transfer from the laboratory to industry. Our funding sources include the Swiss Innovation Agency (Innosuisse), the EU (Eurostars, Horizon 2020), the Swiss National Science Foundation (SNSF) and various private foundations as well as direct funding from industry.

Our core competence is the development of new sensors and measurement methods in biomedical engineering. In particular, we are experienced in skin science and technology: artificial skin models, computer simulations, development of new sensors, etc We benefit from the state-of-the-art infrastructure of the Optoelectronic Research Laboratory (OLAB) that allows the development of demanding prototypes.



C. Aybar



D. Fehr



D. Bajrami



F. Spano



J. Zwicky



M. Hostettler



M. Boldrini



M. Bonmarin



R. Hagen



V. Buff

# 4.1 Lock-in Thermal Imaging for the Characterization of Photothermal Transparent Thin Films

This work explores the use of a novel Lock-in Thermography platform, Calorsito, for the detailed characterization of photothermal thin films. As a high-sensitivity imaging method, Lock-in Thermography enables the detection of subtle thermal signatures, material heterogeneities, and nanoparticle clustering. The Calorsito system integrates multi-wavelength infrared excitation with precise thermal imaging capabilities. Thin films composed of Fe $_3$ O $_4$ , Fe $_3$ O $_4$ @Cu $_2x$ S, and Chlorophyllin were investigated. The device successfully revealed localized heating effects and aggregation patterns. Experimental results demonstrated that average visual transmittance (AVT) was a more critical factor than concentration in determining temperature increase, underscoring the importance of AVT in governing photothermal response and light absorption efficiency.

Contributors: G. Butler, H. Carter, D. Bajrami, S. Shrestha, D. Shi, M. Bonmarin

Partners: NanoLockin GmbH, EMPA, University of Cincinnati

Funding: SNSF Scientific Exchange

Duration: 2024

Photothermal thin films are gaining momentum as a means of converting ambient light into heat, offering promising applications in sustainable energy and smart building integration. Unlike photovoltaics, which depend heavily on direct sunlight, photothermal systems can harvest diffuse light and convert it into thermal energy even under low-light conditions.

In this project, thin films incorporating  $Fe_3O_4$ ,  $Fe_3O_4$ @ $Cu_{2x}S$ , and Chlorophyllin nanoparticles were synthesized.  $Fe_3O_4$  offers strong UV absorption and magnetic properties, while  $Fe_3O_4$ @ $Cu_{2x}S$  benefits from localized surface plasmon resonance (LSPR), granting it broad absorption from UV to near-infrared. Chlorophyllin, a biogenic pigment, is well-suited for visible light absorption and eco-friendly applications.

The films were deposited on microglass slides using spin coating, and their optical and thermal properties were systematically studied. UV-Vis spectroscopy was used to measure absorbance spectra from 300–1000 nm. Thermal behavior was then characterized using the Calorsito VIS-NIR device (NanoLockin GmbH), which enables detection of heat signatures at seven discrete wavelengths ranging from 400 to 940 nm.

Lock-in thermography (LIT) works by modulating incident light and measuring surface temperature changes using an infrared camera. The resulting phase and amplitude maps reveal heat distribution

and highlight inhomogeneities due to particle aggregation or film defects. This high sensitivity technique is especially powerful for nanomaterial analysis, where thermal signals are often subtle.

Experimental results showed strong alignment between UV-Vis absorbance and thermal response. Fe $_3$ O $_4$ @Cu $_{2x}$ S exhibited the highest photothermal conversion, especially at longer wavelengths, due to its LSPR-enhanced absorption. Chlorophyllin demonstrated efficient heating in the visible spectrum, particularly around 400 nm, while Fe $_3$ O $_4$  remained limited in thermal performance except under broad-spectrum white light, where IR contributions play a role.

Temperature increase ( $\Delta T$ ) under white light was inversely correlated with Average Visual Transmittance (AVT). Films with lower AVT values absorbed more light and generated higher temperatures, confirming the trade-off between transparency and thermal performance. Additionally, LIT allowed for the visualization of heat hot spots caused by particle clustering, which are invisible to conventional imaging.

This study validates the Calorsito LIT platform as a versatile and accurate tool for characterizing advanced photothermal materials. Its ability to correlate optical absorption, thermal behavior, and film uniformity makes it well-suited for material screening and optimization in photothermal applications such as energy harvesting, smart coatings, and biomedical devices.

# 4.2 Miniaturized Magnetic Actuation System for Precision Controlled Flow in Medical Environments

This development focuses on the miniaturization and redesign of a magnetic actuation system intended for ultra-precise flow manipulation in highly constrained environments, particularly within the medical field. Building upon the scalable simulation models established in earlier stages of the project, this phase explores the translation of core principles to a system with an internal flow diameter of just 1 mm. The reduction in scale imposed significant design and control challenges, which were overcome through an iterative process involving advanced simulation, prototyping, and integration of high-precision manufacturing techniques.

Contributors: M. Boldrini, V. Buff, G. Boiger

Partners: Confidential Funding: Innosuisse Duration: 2023-2025

Magnetic actuation technologies offer inherent advantages in hygienic applications due to their contactless operation and sealed geometry. However, their scalability to diameters below 1 mm introduces new constraints on magnetic field strength, thermal management, and mechanical tolerances. This research stage focused on adapting previously validated actuation concepts to meet the demands of miniaturized flow systems, with particular attention to energy efficiency, precision control, and dynamic response under varying operational conditions.

The newly developed system leverages a hybrid configuration of permanent magnets and dynamically controlled electromagnetic coils. To address the extreme geometric constraints, customized micro-fabrication strategies were employed alongside redesigned magnetic field paths optimized via high-resolution finite element simulations. These simulations were critical in predicting field interactions, component alignment tolerances, and saturation behaviors at reduced scales (Fig. 1).

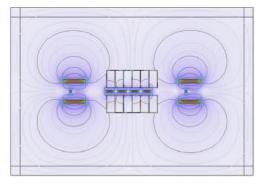


Fig. 1: Magnetic field simulation of the miniaturized configuration.

One key outcome was the identification and mitigation of non-linear force behaviors that become prominent at miniature scale due to boundary effects and increased sensitivity to magnetic misalignment. Control algorithms were refined to compensate for these behaviors, allowing the system to maintain stable operation with minimal overshoot and high repeatability even at sub-millimeter motion ranges. Dynamic simulations were conducted to characterize response times and energy consumption across a range of operational conditions (Fig. 2).

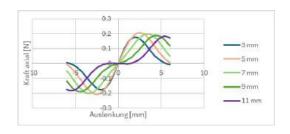


Fig. 2: Simulated force response and displacement curve at 1 mm system scales.

Prototypes of the system demonstrated a strong correlation with simulation predictions, confirming the feasibility of the miniaturized design. The device maintained precise, repeatable actuation in a highly compact footprint, meeting key design criteria for integration into medical platforms requiring sterile, contactless, and highly controlled flow management.

This work represents a substantial step in translating scalable magnetic actuation technology into micro-scale systems suitable for sensitive applications.

### 4.3 Point-of-Care Device for Blood Ammonia Monitoring

Hyperammonemia and its neurological consequences, such as hepatic encephalopathy, affect up to 45% of cirrhotic patients and can lead to coma or death. This project aimed to develop a portable, user-friendly, and cost-effective point-of-care diagnostic device for rapid quantification of ammonia in blood. The device is designed to read a fluorescence-based pH-gradient polymersome assay and is intended to support regular monitoring by healthcare professionals and patients.

Contributors: D. Fehr, J. Zwicky, M. Wyrsch, S. Steiger, R. Hagen,

C. Grossmann, F. Spano, M. Bonmarin

Partners: Versantis AG Funding: Innosuisse Duration: 2022–2025

In this project, a compact point-of-care (POC) diagnostic prototype device was designed and implemented in collaboration with Versantis AG. The device quantifies ammonia in blood by measuring fluorescence changes in a pH-sensitive dye encapsulated within polymersomes developed by Versantis. These vesicles respond to ammonia diffusion by altering their internal pH, which in turn modulates the dye's fluorescence intensity [1].

The optical system was designed to enable stable ratiometric fluorescence detection using a single photodiode and a custom tunable bandpass filter. This configuration allows sequential measurement of reference and signal wavelengths, which helps reduce variability due to sample positioning and component tolerances.

The electronics were adapted to meet the constraints of a portable device. The circuit design was refined to reduce size and improve resistance to electromagnetic interference. A simple user interface was implemented, consisting of physical buttons and a display screen for initiating measurements and reading results. Calibration data and test outputs are stored on a removable SD card, and a graphical interface was developed to support calibration and data visualization via a connected computer.

The fluidic system was designed to minimize user involvement, handle small blood volumes, and ensure consistent mixing with the reagent. Following the displayed instructions, the user loads a pouch containing the reagent into the device, fills a single-use transfer pipette with the blood sample, and inserts the filled pipette into the device. Au-

tomation was achieved using custom-formed blister pouches and a servo-actuated pipette mechanism. Several iterations were made to improve the reliability of sample handling, including adjustments to pipette insertion depth and blister geometry. These refinements helped reduce variability in the assay and improved overall performance. The final prototype, as shown in Fig. 1, allows for ammonia quantification from an 80  $\mu$ L blood sample within seconds, covering a clinically relevant concentration range of 30  $\mu$ M to 800  $\mu$ M. It meets ICH M10 validation criteria and provides a foundation for further development and industrialization of the POC device, with potential to support improved



disease monitoring and patient care.

Fig. 1: Final prototype of the point-of-care testing device for the quantification and monitoring of blood ammonia levels using the assay developed by Versantis.

#### References:

[1] A. Spyrogianni, C. Gourmel, L. Hofmann, J. Marbach, and J.-C. Leroux, "Optimization of an ammonia assay based on transmembrane pH-gradient polymersomes," *Scientific Reports*, vol. 11, no. 1, p. 22032, Nov. 2021.

# 4.4 Innovative 3D printed semi-dry electrode for EEG portable device

This thesis presents the design and development of innovative 3D-printed semi-dry electrodes for EEG signal acquisition. The electrodes integrate a biodegradable hydrogel layer and encapsulated electrolyte droplets that release upon contact with skin moisture, reducing impedance and enhancing signal quality. Fabricated using conductive PLA filament, the design allows for low-cost, customizable production. A compact, portable EEG device with Bluetooth connectivity and a smartphone app was also developed to support real-time data visualization. Initial testing confirmed successful signal acquisition, demonstrating the system's potential for wearable neurotechnology applications. Further work is needed to optimize hydrogel performance and improve long-term reliability.

Contributors: C. Grossmann Aybar, F. Spano

Partners:

Funding: Master's Thesis Duration: 2024–2025

Electroencephalography (EEG) is a non-invasive technique used to record brain activity and plays a critical role in both clinical diagnostics and neuroscience research. Traditional EEG systems rely on wet electrodes, which require the application of conductive gels to ensure good electrical contact with the scalp. Although effective, these systems are often time-consuming to set up, uncomfortable for users, and may cause skin irritation.

Dry electrodes offer a more convenient alternative by eliminating gels, making them easier to apply and better suited for wearable applications. However, they typically exhibit higher skin-electrode impedance and are more prone to motion artifacts, which can reduce signal quality. To overcome these limitations, semi-dry electrodes have emerged as a promising hybrid solution. These electrodes incorporate an internal mechanism that gradually releases a small amount of electrolyte during use, helping reduce impedance while maintaining the simplicity and comfort of dry electrodes. Building on this concept, this project presents an innovative approach to EEG signal acquisition using custom-designed, 3D-printed semi-dry electrodes. The design integrates a biodegradable hydrogel layer and encapsulated electrolyte droplets within a soft polymer matrix. When the electrode comes into contact with skin moisture, the hydrogel degrades, triggering a controlled release of the electrolyte—enhancing electrical connectivity without the need for external gels or complex preparation.

The electrode body was fabricated using conductive PLA filament and 3D printing, enabling low-cost production and precise control over geometry. Complementing the electrode design, a compact EEG recording device was developed, featuring a rechargeable battery, Bluetooth Low Energy (BLE) connectivity, and a smartphone app for real-time signal display and data storage. The result is a portable, user-friendly system that supports flexible EEG acquisition beyond traditional laboratory environments.

Initial testing confirmed successful signal acquisition and integration between the electrodes and recording device. While further refinement is needed—particularly in optimizing impedance and improving hydrogel durability—the system demonstrates strong potential for future applications in wearable, accessible neurotechnology for both clinical and consumer use.

#### Literature:

[1] G. L. Li et al., *J. Neural Engineering*, Vol. 17, 2020.

[2] J. Rosell et al., *IEEE Transactions on Biomedical Engineering*, Vol. 35, 33–36, 1988.

# 4.5 Replicating fingerprints in Artificial Skin Models by 3D Printing

In this work, we are implementing the replication of fingerprints into artificial skin models generated by 3D DLP printing process. On the basis of the use of specific soft polymeric resins, we can directly print fingerprints onto a skin model mimicking the real human skin topography.

Contributors: B. Heer, F. Spano & M. Bonmarin

Partners: Université de Lausanne (UNIL) – Ecole des Sciences Criminelles (ESC)

Funding: Student Project Duration: 2024–2025

3D printing has revolutionized many fields, from medicine and aerospace to art and design. One of the most fascinating and potentially controversial applications of this technology is the reproduction of fingerprints. Fingerprints, unique to everyone, have long been considered an infallible method of personal identification. However, with advances in technology, the possibility of duplicating these fingerprints raises technical and ethical questions. This work explores the different facets of fingerprinting using 3D printing. We begin with an overview of the 3D printing technologies available and their recent evolution. We look at the specific techniques used to capture and reproduce fingerprints, as well as the materials used to create accurate replicas. We also look at the potential applications of this technology, such as in the field of forensics, with our partner at the School of Criminal Justice (University of Lausanne).

In the framework of this collaboration, the project aims at creating first a series of stamps with various patterns mimicking the fingerprints. We will

study the deformation capabilities of the selected materials bearing the pattern (e.g. shearing, embossing) allowing the material to adapt its shape when applied on a textured surface simulating fingerprints in crime scene. In addition to mechanical properties, we will study the wetting properties of employed resins with variable degrees of hydrophobicity and oleophobicity. First, we will focus on the development of a relevant protocol for the realization of the stamp prototypes, especially the choice of the deformable materials. A preliminary work could focus on the design of specific patterns which may be reproduced using rigid stamps as models for molds (such stamps being provided by ESC/UNIL). The ability to reproduce unique biometric characteristics poses major challenges in terms of privacy protection and data security. The School of Criminal Justice will help us to discriminate the current regulations and the measures that could be put in place to govern the use of this tech-

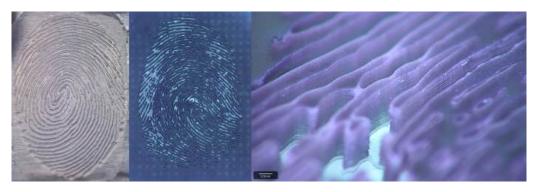


Fig. 1: Illustrations of various artificial skin models mimicking the fingerprints.

# 4.6 Development of a Multimodal Optical Measurement System for Bilirubin Quantification and Differentiation

This work presents an optical approach for distinguishing free, bound, and conjugated bilirubin, relevant for improved jaundice diagnostics. A custom device was developed to perform absorbance, fluorescence, anisotropy, and bleaching measurements using a laser diode and tailored electronics. Measurements on synthetic bilirubin samples revealed distinct optical signatures for each form, with fluorescence and anisotropy proving particularly effective in identifying bound bilirubin. The results establish a foundation for accurate, point-of-care bilirubin analysis.

Contributors: J. Zwicky, D. Fehr, M. Bonmarin

Partners: Institute of Chemistry and Biotechnology (ZHAW)

Funding: Master's degree programme

Duration: 2024-2025

Bilirubin is a yellow pigment formed during red blood cell degradation. Due to its low solubility in blood, it binds to the transport protein albumin before being conjugated in the liver to increase its water solubility for excretion. Elevated levels of free bilirubin can lead to jaundice and, in severe cases, neurological damage, particularly in neonates. Conventional clinical methods measure only total and conjugated bilirubin, without differentiating the free and bound forms – limiting diagnostic precision.

This work presents a novel optical system designed to quantify and differentiate free, bound, and conjugated bilirubin. The measurement system combines absorbance, fluorescence, fluorescence anisotropy, and photobleaching techniques

to characterise the optical properties of different bilirubin types. A custom-built device integrates a laser excitation source, optical modules and centralised control electronics, with data processed via a Python-based software interface.

Measurements on synthetic bilirubin samples demonstrated concentration-dependent absorbance and fluorescence responses, with bound bilirubin showing a distinct fluorescence signature. Anisotropy measurements highlighted molecular binding effects, while photobleaching dynamics revealed differences in stability among bilirubin forms. The results validate the feasibility of a multimodal approach for bilirubin analysis and establish a foundation for future point-of-care diagnostic systems.

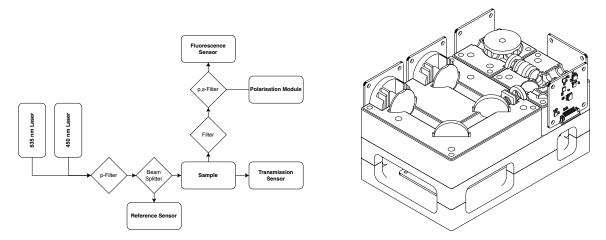


Fig. 1: Left: Functional diagram of the optical setup with L-shaped geometry. A laser excites the sample, while another laser compensates for matrix absorbance. Reference and transmission sensors enable ratiometric absorbance measurements. Fluorescence is filtered, polarised, and detected by a sensitive sensor. Right: Isometric view of the assembled measurement device showing key optical and electronic components.

# **5 Building Simulation**

Buildings affect our well-being, productivity, and various social interactions. Much of our energy is used in buildings, and through utilization of solar energy and environmental heat, modern buildings have become energy producers themselves. Large volumes of information, goods and people move around buildings. Data is continuously collected using sensors and measurement technology; simulations and control technology are used to ensure that all these processes can be optimally supported and controlled in an increasingly digital world.

At ICP, we support the digitalization in the building sector with computer simulations for physical-technical processes. Our contributions extend from the early through to the detailed planning phase all the way to the operation of the buildings. We have access to a large number of simulation tools and design our own algorithms where necessary. We use measurement technology to validate the simulations, determine material parameters and generate output data for predictive simulations.

In 2022, the Swiss Building Simulation Association was established, which has transferred its management to the ICP (www.gebaeudesimulation.ch). The association brings together leading planning offices from the fields of construction and energy planning to jointly promote physical simulations in the construction industry. It currently has more than 50 members.



A. Drigatti



C. Fachin



D. Bernhardsgrütter



F. Schranz



M. Schmid



E. Linder



A. Witzig



M. Roos



Z. Bratsos

## 5.1 ThermoPlaner3D - Building energy evaluation from largearea 3D thermography

ThermoPlaner3D develops large-scale, detailed 3D building energy assessments from multiperspective thermographic images, creating a new quantitative planning basis as well as a marketing tool for energy suppliers.

Contributors: M. Battaglia, E. Comi, D. Meier, F. Schranz Partners: FHNW, Considerate AG, BSF Swissphoto

Funding: Innosuisse Duration: 2021–2024

The increase of the renovation rate in the building sector is a central component in the reduction of the energy demand of Switzerland. The Thermo-Planer3D project is developing an innovative product that enables energy supply companies (EVUs) to support the energy transition and profit from it at the same time.

While today energetic assessments of buildings are mainly done for single objects, there is a lack of tools to offer owners a low-threshold initial assessment of their building and to show them the potential of a refurbishment. The ThermoPlaner3D project aims to provide the necessary quantitative basis for an entire urban area with a single measurement flight using multiperspective thermal images from a remote sensing aircraft.

A first test flight was carried out in Grenchen before the start of the project in late winter 2021. With SWG, the utility company of Grenchen, a pilot customer for feedback is involved. Valuable insights were gained from the first test flight, which could be further refined in a second test flight in the winter of 2023 in Aalen in Baden-Württemberg.

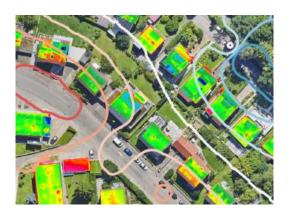


Fig. 1: Roof temperatures and microclimate of a district.

The ICP is responsible for the scientific monitoring of data acquisition using infrared measurement technology and attempts to improve the evaluation and correction of the data using known and new approaches. We are also contributing our expertise in building simulation in order to be able to make statements about the annual consumption of the respective buildings from point measurements of the external temperatures of the building envelope.

Figure 1 shows the roof temperatures of buildings including the microclimate temperature ranges. A heat transmission value (U-value) is then estimated from the averaged roof temperature using a simple thermal model of the roof. The microclimate can be calculated as a by-product of a thermography flight using the TURN algorithm (Thermal Urban Road Normalization).

When analysing the flight data, it was found that the calculated U-values deviated significantly from the actual values in some cases. Consequently, a comprehensive sensitivity analysis was carried out. The results in Figure 2 show that the measured temperatures must be very accurate for a good U-value estimate and that the weather conditions during the flight are extremely important.

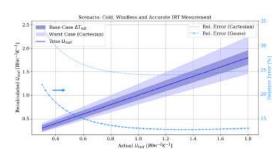


Fig. 2: The sensitivity analysis shows the expected deviation in the U-values under ideal conditions.

## 5.2 Crowd management for major events through faster-thanreal-time simulation of pedestrian flow

Simulations of pedestrian flow are widely used to design guidelines during the planning of large events. We examine how faster-than-real-time (FTRT) simulations of pedestrian flow can contribute to dynamic control strategies of the crowd in order to ensure safety during the event. For this purpose we use a continuous model for pedestrian flow, which is solved by the finite element method. This approach enables efficient simulations at low computation time, making it ideal for real-time crowd management at large events.

Contributors: D. Bernhardsgrütter, M. Schmid

Partners:

Funding: Digital Futures Fund (ZHAW digital)

Duration: 2024

Crowd management is crucial for large events such as concerts, festivals or public demonstrations. The safety and efficiency of pedestrian flow during these events are paramount, as even minor disruptions can lead to significant risks including crowd crushes. Consequently, the ability to predict and manage pedestrian crowds in real-time has become increasingly important for event organizers and emergency services.

To effectively manage crowds, simulations that operate faster than real-time are necessary. Such simulations allow planners to anticipate potential issues and adjust strategies before problems arise. For instance, during an evacuation, being able to predict the flow of people towards different exits can inform decisions about opening or closing certain pathways, deploying additional staff, or broadcasting specific instructions. The capability to simulate these scenarios quickly and accurately can make the difference between a controlled evacuation and a chaotic situation.

In this context, we use a continuous model [1, 2] to simulate the pedestrian dynamics. The model is derived by regularizing Hughes' model of pedestrian flow [3] allowing the solution by the finite element method. Unlike agent-based models, which track individual persons within the crowd, continuous models treat the pedestrian density  $\varrho$  as a continuous field. This approach is more scalable and efficient for representing large numbers of people, making it ideal for large events. In Fig. 1 the density  $\varrho$  is shown for a simulation of the "Winterthurer Musikfestwochen", which is a festival event taking place yearly in the old town of Winterthur with several thousands of attendees.

We demonstrate the capability to simulate pedestrian flow faster than in real-time for the Win-

terthurer Musikfestwochen. We define the FTRT ratio as the quotient of the simulated evacuation time  $t_{\rm eva}=757$  s and the physical computation time  $t_{\rm sim}=18$  s. Thus even for large events with tens of thousands of attendees, FTRT ratios as high as  $t_{\rm eva}/t_{\rm sim}=42$  are feasible. The simulations were performed on a laptop with a single Intel i7 CPU at 1.8 GHz.

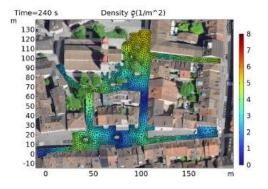


Fig. 1: Simulation results for the evacuation of the "Winterthurer Musikfestwochen". The pedestrian density  $\varrho$  (in pedestrians/m²) at t=240 s is shown.

As a next step, the objective is to validate the model with greater precision by comparing the simulations with empirical data obtained from events and with simulations from agent-based models.

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- [1] M. Schmid et al., Faster-than-real-time Simulation of Multi-group Pedestrian Flow, in Traffic and Granular Flow '24, Springer International Publishing (accepted for publication)
- [2] R. Axthelm, in Traffic and Granular Flow '15, edited by V.L. Knoop, W. Daamen (Springer International Publishing, 2016), pp. 233–240
- [3] R.L. Hughes, Transportation Research Part B: Methodological 36, 507 (2002)

## 5.3 EFFIWAG: Efficiency potential of replacing the heat distribution system

The market share of heat pumps is steadily increasing, leading to higher electricity demand, especially during the winter months. In the EFFIWAG project, we analyse various measures to reduce the electricity consumption of heat pumps in existing buildings. Heat pumps operate most efficiently at low supply temperatures, which is why we are investigating the potential of low-temperature radiators. Simulations of five buildings in Zurich show that replacing radiators with low-temperature radiators reduces energy consumption and CO<sub>2</sub> emissions in the unrenovated state by 30%.

Contributors: F. Schranz, J. Bruderer, L. Meier, A. Witzig

Partners: Lemonconsult AG

Funding: BFE, AWEL, Dr.-Stephan-à-Porta-Stiftung

Duration: 2023–2025

A heat pump operates most efficiently when only a small temperature lift is required. For buildings with heat pump heating systems, this means efficiency increases as the flow temperature of the heat distribution system decreases. However, existing buildings typically use radiators requiring flow temperatures of 60°C or higher. This results in a low COP (Coefficient of Performance) of just 1.6 to 1.8 for air-to-water heat pumps during winter months. In this project, we investigate how replacing the heat distribution system combined with various retrofit measures affects the energy consumption and CO<sub>2</sub> emission of existing buildings. Our focus lies on the potential of low-temperature radiators, as installing underfloor heating in occupied buildings is often impractical.

To this end, we modelled five buildings in the Zurich area using IDA-ICE software (see Fig. 1). For each building, three retrofit states were analysed: a reconstructed original state, a partial

retrofit with new windows and insulation of the cellar ceiling and attic, and a full retrofit including facade insulation. These states were combined with three heat distribution systems (radiators at 60°C flow temperature, low-temperature radiators at 40°C, and underfloor heating at 35°C), and heating energy consumption was calculated. Lemon Consult determined the specific COPs of the heat pumps and computed the grey energy generated during retrofitting.

The results demonstrate that replacing radiators with low-temperature radiators in unretrofitted buildings reduces energy consumption and CO2 emissions (from production and operation) by 30%. Further significant reductions in energy use and CO2 emissions are achievable only through comprehensive full retrofits. A detailed article about this project was published in the technical journal HK-Gebäudetechnik [1].



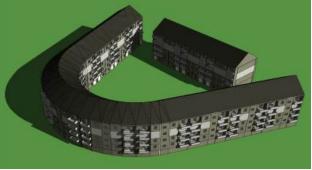


Fig. 1: Two of the five buildings modelled with IDA-ICE are shown. To save computation time, the third floor of the building complex on the right is omitted, and instead, the second floor is duplicated.

#### References:

[1] B. Vogel, Runter mit der Vorlauftemperatur, HK-Gebäudetechnik 3, 2025.

## 5.4 Energy saving with intelligent shading systems

This study investigates the ecologically optimized operation of shading systems. Using ray-tracing simulations, the amount of solar energy entering a room is calculated. The subsequent analysis reveals the savings potential: solar blinds contribute to overheating protection in summer by providing shade. During the colder months, sunlight is allowed to enter through the windows whenever possible, so that passive solar gains support heating.

Contributors: A. Ehrler, A. Witzig

Partners: Bühler und Scherler AG, Schenker Storen AG

Funding: Bachelorarbeit

Duration: 2025

Currently, buildings account for around 40 percent of Switzerland's final energy consumption. An important and well-controllable heat source is solar radiation through windows. Short-wave sunlight passes through the windows and generates heat, while long-wave thermal radiation from inside is reflected back by the windows and remains in the building (greenhouse effect). Therefore, a smart shading system can lead to significant energy savings.

The system works differently depending on the season: in summer, optimal shading helps prevent overheating. Unnecessary heating of the interior by direct sunlight is avoided, thus reducing the need for resource-intensive active cooling. In winter, on the other hand, passive solar gains are maximized, reducing the building's heating demand.

The simulations are primarily conducted in 2D using the ray tracing method [1]. They take into account the position of the sun as well as the type and position of the shading devices. In addition, the irradiated power is calculated based on the orientation of the window and the sun's azimuth angle. Various shading systems and control algorithms are compared.

This bachelor's thesis is oriented toward an industrial application that supports many types of shading systems and has the potential to lead to substantial energy savings across Europe.

#### References:

[1] Comsol Ray Optics Module, *Application Example* https://www.comsol.de/model/vdara-causticsurface-18531



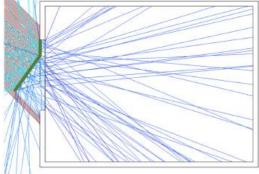


Fig. 1: Top: Exemplary representation of a retractable awning (image generated using AI). Bottom: 2D ray tracing in a cross-section of the shading system and the interior space behind it. The solar rays are scattered by the fabric (green contour). The simulation calculates how much of the scattered sunlight enters the room. Dark red lines: incoming solar rays; blue lines: scattered light. The image illustrates the simulation principle using a reduced number of rays. A convergence analysis has shown that a higher ray density is required for accurate simulations.

## 5.5 Simulation of Efficient Heating Systems in Churches

Heating a church efficiently is a challenging task. However, a concept that has won multiple awards promises a cost-effective solution that meets the specific requirements and consumes only a fraction of the energy during operation. The simulations in this project can be used to visualize how the system works and help convince sceptics. The air-based heating system holds great potential for future renovations.

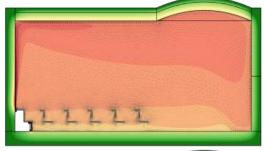
Contributors: C. Tello, A. Witzig
Partners: Kegel Energy Systems

Funding: ICP

Duration: 2023-2025

Unlike residential or office buildings, churches are not always kept at a constant set temperature. The heating is only turned on when needed. This is also true for traditional heating systems, which require radiators to operate at very high temperatures (typically: 60°C) to release enough energy into the space.

The innovative concept studied here is based on generating an airflow via a heat exchanger with fans, which brings the warm air into the room. The required supply temperatures for the heating water are much lower (typically: 27°C). This is a major advantage when using heat pumps, as the smaller temperature differences make the heating devices operate much more efficiently. Additionally, the heat is distributed better in the interior, avoiding hot air columns rising all the way to the ceiling. Instead, the interior warms up more evenly. In particular, the heating system demonstrates advantageous dynamics, as primarily the air is heated, and not the massive stone floor or walls. Besides better efficiency, retrofitting the heating system can also be more cost-effective and quicker to implement. This work simulates a comparison between a traditional heating system and the novel air-based heating system. The results aim to convince sceptics. For the broader adoption of this energetically superior and innovative system, it is important not only that the physics of the system is understood, but also that it can be well communicated through simulations.



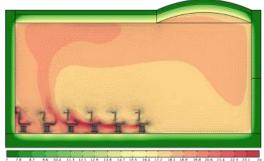


Fig. 1: Comparison between the efficient new air-based heating system (top) and the traditional heating system, which has a radiator under each pew (bottom). The simulations, shown in a longitudinal section of the church, calculate airflow as well as the temperature distribution in the interior and the walls.

#### References:

[1] B. Kegel, Energieschleuder Kirche: Zürcher Kirche zeigt, wie es besser geht, https://energeiaplus.com/2024/11/26/energieschleuder-kirche-zuercher-kirche-zeigt-wies-anders-geht/

# 5.6 Massive parallelization for the simulation of decentralized energy systems

In a research project together with the provider of the simulation software Polysun, a framework was implemented that offers massive parallelization of building technology simulations. By integrating a multi-objective optimization algorithm we are able to automatically determine an optimal dimensioning of the system's components.

Contributors: M. Battaglia, A. Drigatti, E. Linder, F. Schranz, A. Witzig

Partners: Vela Solaris AG Funding: Innosuisse Duration: 2023–2025

The Polysun software enables the simulation of decentralized energy systems. In practice, users typically define an energy system and settle for the first plausibly functioning configuration, as further optimization must be performed manually.

To address this problem, our first-generation prototype introduced a frontend that allows users to individually configure parameters for multi-simulations across a number of given system choices, leveraging massive parallelization to accelerate the process. This frontend also provides tools to analyse results, focusing on key parameters such as CO<sub>2</sub> emissions, costs, and self-consumption fraction, thereby assisting users in selecting the optimal system.

Building on this foundation, the second generation of our prototype automates the search for the optimal system, eliminating the need for user input. The framework now supports the entire workflow:

it transfers specific settings from the Polysun desktop application to a web-based multi-simulation engine, where the optimization is performed automatically. The components which are optimised are chosen automatically, and we developed algorithms that determine appropriate boundary conditions and optimal step sizes for these components. To efficiently identify optimal solutions, we implemented a genetic algorithm for multi-objective optimization. This algorithm intelligently explores the solution space and approaches the Pareto front which is the limit of the physically possible solutions. It calculates five generations of twenty points each. With every new offspring the likelihood of the points being closer to the Pareto front increases as shown in Fig. 1.

As the optimal system we identify a system which lies on the Pareto front and has both lower CO<sub>2</sub> emissions and lower costs than the default system.

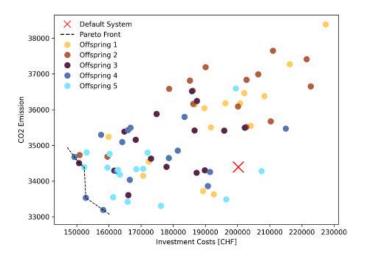


Fig. 1: A system with a ground source heat pump and PV is optimized for CO<sub>2</sub>-emissions and investment cost. The figure shows how the multi-opjective-optimization algorithm approaches the Pareto front. With every offspring the points move closer to the Pareto front.

# 5.7 Thermo chemical networks (TCN) for residential heat demand coverage

In this topic, we address the coverage of residential heat demand using thermochemical networks (TCN). The ICP contribution focuses on modeling the thermal aspects of such networks, for example by using a heat pump to regenerate salt solutions during the summer. ICP collaborates closely with IEFE, which possesses extensive expertise in salt solutions and related chemical properties, such as specific heat capacity, solubility, and boiling temperatures. TCNs can serve as seasonal thermal energy storage systems and may help to bridge the winter electricity gap. This research is conducted within the framework of the PEDvolution and UPchange projects.

Contributors: E. Linder, F. Schranz, A. Witzig Partners: S. Danesi, T. Bergmann (IEFE)

Funding: SNF Duration: 2025–2027

The energy demand for residential heating, hot water, and air conditioning in Switzerland accounts for almost 40 % of the country's total energy consumption. A major challenge is how to meet this demand during winter, when the availability of electric energy is limited in Switzerland and neighboring countries. Thermochemical networks (TCNs) offer the opportunity for long-term energy storage with a higher storage density compared to conventional thermal storage systems based on water. This technology could help close the winter electricity gap and decarbonize residential heating by transferring excess energy from summer to winter.

A thermochemical network operates on the principles of an absorption heat pump. In such a system, a salt solution acts as the absorbent and is circulated from the consumer side (evaporator-absorber) to the regenerator (desorber-condenser). On the evaporator-absorber side, water vapor is added as a refrigerant and absorbed by the concentrated salt solution, releasing the chemical potential (stored ex-

ergy) as useful heat. In the desorber-condenser, the salt solution is heated, causing water to evaporate and increasing the concentration of the salt solution. The concentrated solution is then pumped back to the evaporator-absorber, completing the cycle. A schematic overview is provided in Fig. 1. The potential of this technology has already been explored in practice by installing a demonstrator in a greenhouse [1].

This work aims to realize a TCN simulation and conduct a case study for the Hard community in Winterthur. The community has installed photovoltaic (PV) panels, and the electricity generated can be used to operate a heat pump for the desorption of the salt solution during summer.

The research questions addressed in this work include: How much salt solution is required to cover the heating demand of the Hard community? What type of heat pump and PV area are needed for this purpose? Does TCN technology provide a viable solution for meeting the community's heating demand?

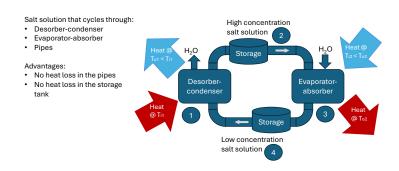


Fig. 1: Schematic overview for a TCN.

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# **Appendix**

## A.1 Scientific Publications

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## A.5 Student Projects

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- M. Andres, J. Hinnen, *Entwicklung eines LED-basierten Sonnensimulators für die Solarzellenforschung*, Betreuer: K. Pernstich, Bachelorarbeit im Studiengang Systemtechnik.
- J. AUS DER AU, R. MÜLLER, *Measuring the Skin Thermal Diffusivity In-vivo*, Betreuer: D. Fehr, Projektarbeit im Studiengang Systemtechnik.
- S. BOLLETER, R. GEHRING, S. EMALE, *Microwave Hyperthermia for Cancer Treatment*, Betreuer: M. Bonmarin, Bachelorarbeit im Studiengang Systemtechnik.
- Y. CORNAZ, *Erdreichanbindung für Heiz- und Kühlsysteme ST*, Betreuer: A. Witzig, Bachelorarbeit im Studiengang Elektrotechnik.
- A. DRIGATTI, L. KELLER, *Data Analysis for Blood Flow Sensor*, Betreuerin: E. Knapp, Bachelorarbeit im Studien-gang Data Science.
- A. EHRLER, *Intelligente Beschattungssysteme ET*, Betreuer: A. Witzig, Bachelorarbeit im Studiengang Elektrotechnik.
- M. EUGSTER, *Praxissemester BSc Medizininformatik*, Betreuer: M. Bonmarin.
- Q. FITZI, M. LUPO, *Entwicklung eines integrierten Blutvolumensensors für ein PoC-Messgerät*, Betreuer: D. Fehr, Bachelorarbeit im Studiengang Systemtechnik.
- A. GARCIA BUSTOS, Simulation of light-induced acoustic interactions with inner ear structures via plasmonic nanoparticle stimulation using Finite Element Methods (FEM), Betreuer: M. Jazbinsek, M. Bonmarin, Vertiefungsarbeit Masterstudiengang.
- M. GNOS, M. WICKIHALDER, *Effiziente Heizungsanlage in einer Kirche*, Betreuer: A. Witzig, Bachelorarbeit im Studiengang Systemtechnik.
- R. HAUS, *Upscaling of perovskite solar cells: from cell to module*, Betreuer: E. Knapp, E. Comi, Projektarbeit im Studiengang Systemtechnik.
- R. Haus, *Simulation and Optimization of Perovskite Solar Modules: A Software-Driven Approach*, Betreuer: E. Knapp, E. Comi, Bachelorarbeit im Studiengang Systemtechnik.
- I. HÄUSLER, *Thermal Imaging Monitoring of Sweat Glands*, Betreuer: M. Bonmarin, Masterarbeit MSE Medical Engineering.

- B. HEER, *Flexible multidirectional capacitive angle sensors for spine monitoring*, Betreuer: F. Spano, Vertiefungsarbeit Masterstudingang.
- B. HEER, DermatoTherma: Development of an artificial skin model for the characterization of radio-frequency heating, Betreuer: F. Spano, Bachelorarbeit im Studien-gang Systemtechnik.
- N. Kabir, *Substrates for broadband terahertz time-domain spectroscopy of thin films*, Betreuerin: M. Jazbinsek, Vertiefungsarbeit Masterstudiengang.
- N. Kabir, *Characterizing the spatial profile of deep UV light source*, Betreuer: M. Bonmarin, Vertiefungsarbeit Masterstudiengang.
- T. KALONGI, *Flame-based synthesis for wound dressing applications*, Betreuer: F. Spano, Masterarbeit MSE Medical Engineering.
- G.-L.-LIBERATO, S.-SUVAJAC, *Development and implementation of pressure sensors based on solid liquid composites*, Betreuer: F. Spano, Bachelorarbeit im Studien-gang Systemtechnik.
- J.T. LINK, *Praxissemester BSc Medizininformatik*, Betreuer: F. Spano.
- S. MOHAMMAD, V.K. QUACH, *Perovskite Solar Cells*, Betreuer: W. Tress, Bachelorarbeit im Studiengang Informatik.
- C. MÜNTENER, G. BURGER, *Modellierung eines Wohnraums in Matlab/Simscape für die Optimierung von Energiesystemen*, Betreuer: A. Witzig, Bachelorarbeit im Studien-gang Systemtechnik.
- A. OETSEN, *Development of an artificial intervertebral disk based on solid liquid composites*, Betreuer: F. Spano, Bachelorarbeit in Systems Engineering, Northeastern University USA.
- D. Shanmugathas, *Praxissemester BSc Medizininformatik*, Betreuer: M. Bonmarin.
- A. SUTHESAN, Praxissemester BSc Medizininformatik, Betreuer: D. Fehr.
- A. Schaufelberger, *Microstructure Reconstruction Algorithms for the Catalyst Layer in Fuel Cells*, Betreuer: R. Schärer, Projektarbeit im Studiengang Informatik.
- R. Schwarz, *Simulation of multi-group pedestrian flow*, Betreuer: M. Schmid, Bachelorarbeit im Studiengang Systemtechnik.
- S. Steiger, *A Quantitative Train-of-Four Monitoring Device*, Betreuer: M. Bonmarin, Bachelorarbeit im Studiengang Systemtechnik.
- P. TEREFE, T. VOLLENWEIDER, *Red Blood Cells Monitoring and Preservation*, Betreuer: D. Fehr, Projektarbeit im Studiengang Systemtechnik.
- P. TEREFE, T. VOLLENWEIDER, *Optimization and Characterization of an Optical Sensor Concept to Monitor Supercooled Blood*, Betreuer: D. Fehr, Bachelorarbeit im Studiengang Systemtechnik.
- N. Wartmann, *Microstructure Reconstruction Algorithms for the Catalyst Layer in Fuel Cells (ST)*, Betreuer: R. Schärer, Bachelorarbeit im Studiengang Informatik.
- M. WYRSCH, *Development of a versatile wet-spinning system for multi-layered polymer fibers*, Betreuer: F. Spano, Vertiefungsarbeit Masterstudingang.
- M. WYRSCH, *Fiber-based strain sensors*, Betreuer: M. Bonmarin, Bachelorarbeit im Studiengang Systemtechnik.

J. ZWICKY, Development of a Multimodal Optical Measurement System for Bilirubin Quantification and Differentiation, Betreuer: D. Fehr, Masterarbeit MSE Photonics.

## A.6 Teaching

- M. BATTAGLIA, Physics Engines, FS25, Bachelor of Science.
- D. BERNHARDSGRÜTTER, Lineare Algebra 1 für Systemtechnik, HS24, Bachelor of Science.
- D. BERNHARDSGRÜTTER, Lineare Algebra 2 für Systemtechnik, FS25, Bachelor of Science.
- D. BERNHARDSGRÜTTER, Analysis 1 für Wirtschaftsingenieurwesen, HS24, Bachelor of Science.
- D. BERNHARDSGRÜTTER, Analysis 2 für Wirtschaftsingenieurwesen, FS25, Bachelor of Science.
- M. BONMARIN, Physik für Systemtechnik 1 Vorlesung, HS24, Bachelor of Science.
- M. BONMARIN, HealthTec Summer School Inventing next generation medical devices: From clinic immersion to MVP & business plan, FS24, Master of Science in Engineering.
- M. BONMARIN, Medical Market Access, HS24, Master of Science in Engineering.
- D. Fehr, Grundlagen der Elektrotechnik und Digitaltechnik für Informatik Praktikum, HS24, Bachelor of Science.
- D. FEHR, Physikalische Grundlagen der Sensorik Thema Elektronik, HS24, Bachelor of Science.
- D. Fehr, *Photonics EVA Thermography, FS25*, Master of Science in Engineering.
- D. Fehr, Thermal Devices in Medicine, FS25, Bachelor of Science.
- T. HOCKER, *Physik 1 für Aviatik und Mobility Science, HS24*, Bachelor of Science.
- T. HOCKER, Physik 2 für Aviatik und Mobility Science, FS25, Bachelor of Science.
- T. HOCKER, Projektmodul 1 für Aviatik, HS24, Bachelor of Science.
- T. HOCKER, Projektmodul 2 für Aviatik, FS25, Bachelor of Science.
- T. HOCKER, *Thermische Energiesysteme*, FS25, Bachelor of Science.
- M. JAZBINSEK, *Physik 1 für Maschinentechnik und Energie- und Umwelttechnik Vorlesung & Praktikum HS24*, Bachelor of Science.
- M. JAZBINSEK, *Physik 2 für Maschinentechnik und Energie- und Umwelttechnik Vorlesung & Praktikum FS25*, Bachelor of Science.
- M. JAZBINSEK, Photonics EVA Terahertz Spectroscopy, FS25, Master of Science in Engineering.
- C. Kirsch, Analysis 1 für Systemtechnik, HS24, Bachelor of Science.
- C. KIRSCH, Analysis 2 für Systemtechnik, FS25, Bachelor of Science.

- C. KIRSCH, Analysis 3 für Systemtechnik und Elektrotechnik, HS24, Bachelor of Science.
- C. KIRSCH, Numerik für Systemtechnik und Elektrotechnik, FS25, Bachelor of Science.
- C. Kirsch, *Intensivkurs in Mathematik, Sommer 24*, Studieninteressierte.
- E. KNAPP, Modellierung komplexer Systeme MKS, HS24, Bachelor of Science.
- E. KNAPP, Numerik, FS25, Bachelor of Science.
- E. LINDER, Lineare Algebra 2, FS25, Bachelor of Science.
- P. MARMET, Mathematik: Analysis 1 für Aviatik, Vorlesung und Praktikum, HS24, Bachelor of Science.
- P. MARMET, Mathematik: Analysis 2 für Aviatik, Vorlesung und Praktikum, FS25, Bachelor of Science.
- K. Pernstich, *Physik: Grundlagenprojekt 1 für Verkehrssysteme, HS24*, Bachelor of Science.
- K. Pernstich, *Physik: Grundlagen der Elektrotechnik und Digitaltechnik, Vorlesung und Praktikum, Studiengang Informatik, HS24*, Bachelor of Science.
- K. PERNSTICH, Physik: Grundlagenprojekt 2 für Verkehrssysteme, FS25, Bachelor of Science.
- K. PERNSTICH, *Photonics EVA Quantum Dot Downconversion, FS25*, Master of Science in Engineering.
- K. PERNSTICH, Data Science: Internet of Things for Data Science, FS25, Bachelor of Science.
- K. PERNSTICH, Physik: Physics Engines, Studiengang Informatik, FS25, Bachelor of Science.
- B. RUHSTALLER, Applied Photonics FS25, Master of Science and Engineering.
- B. RUHSTALLER, Advanced Thin Films HS24, Master of Science and Engineering.
- F. SCHRANZ, A. WITZIG, Naturwissenschaften für Medizininformatik, FS24, Bachelor of Science.
- F. SCHRANZ, Grundlagen der Elektrotechnik und Digitaltechnik für Informatik Praktikum, HS24, Bachelor of Science.
- F. SCHRANZ, *Physics Engines, FS25*, Bachelor of Science.
- J. O. SCHUMACHER, Lineare Algebra 2, FS25, Bachelor of Science.
- J. O. SCHUMACHER, Wind-, Wasserkraft, Sektorkopplung, synthetische Treibstoffe, FS25, Bachelor of Science.
- J. O. Schumacher, *Multiphysics Modelling and Simulation, FS25*, Master of Science in Engineering.
- W. TRESS, Physik 1 für Maschinentechnik, HS24, Bachelor of Science.
- W. TRESS, Physik 2 für Maschinentechnik, FS25, Bachelor of Science.
- W. TRESS, Physics on Micro and Nano Scale, HS24, Master of Science in Engineering.

- A. WITZIG, Physik 3, Studiengang Verkehrssysteme, HS24, Bachelor of Science.
- A. WITZIG, *Physik 3, Studiengang Systemtechnik, FS25*, Bachelor of Science.
- A. WITZIG, Wind-, Wasserkraft, Sektorkopplung und synthetische Treibstoffe, Studiengang Energie und Umwelttechnik, FS25, Bachelor of Science.

## A.7 Spin-off Companies



www.fluxim.com

Fluxim is a provider of device simulation software and measurement hardware to the display, lighting and photovoltaics community worldwide. Our principal activity is the development and the marketing of the simulation software SETFOS and LAOSS, as well as the all-in-one characterization platform PAIOS. SETFOS was designed to simulate light propagation and charge transport in large-area opto-electronic devices such as organic light-emitting diodes (OLEDs) and solar cells while PAIOS measures the dynamic opto-electrical response in time and frequency domain which supports the determination of material parameters. Our R&D tools are used worldwide in industrial and academic research labs for the development of devices and semiconducting materials with improved performance as well as the study of device physics.



www.coatmaster.ch

Coatmaster AG (formerly known as Winterthur Instruments) develops measurement systems for fast non-contact and non-destructive testing of industrial coatings. These measurement systems can be used to determine coating thicknesses, material parameters, e.g. porosity and contact quality, to detect delamination, for example. The system is based on optical-thermal measurements and works with all types of coating and substrate materials. Our measurement systems provide the unique opportunity of non-contact and non-destructive testing of arbitrary coatings on substrates.



www.nanolockin.com

NanoLockin is developing the new benchmark technology for the detection and analysis of nanoparticles in all kinds of products. The company won the Fribourg Innovation Award in 2018.

## A.8 Laboratory Infrastructure

An often-underestimated aspect of the development of physical simulation models is their validation and the associated improvement cycle. In terms of effort, this is often much more than a few simple experiments to match the simulation. Instead, this part of the multiphysics development process is the actual link between theoretical development and operational reality. Validation efforts and the associated necessary model improvement cycle can account for up to 60of the project scope. Accordingly, it is important to give this area its appropriate strategic importance. Maintaining or expanding the capabilities of a validation laboratory is therefore important.

### Process laboratory for organic electronics

Since 2012, the centerpiece of this laboratory has been a glove box with nitrogen atmosphere and integrated vacuum chamber for device fabrication by means of thermal evaporation of organic semiconductors and metals. A second box was installed in 2020. Thin films can also be produced from solutions using the spin-on process, and chemistry chambers are available for measurement and sample preparation. The laboratory has measuring methods for determining the optical, electrical and thermal properties of the components.

## **Electronics laboratory**

The electronics lab allows us to efficiently develop, fabricate, and characterize prototypes for R&D projects with our industrial partners. It allows us to validate our simulation models on real systems and it enables us to use specialized instrumentation and sensor technology for the experimental setups in our other laboratories. Finally, students also benefit from the capabilities of our electronics lab, with a focus on rapid prototyping. Our lab meets these demands with a well-balanced basic equipment, such as SMD-capable soldering workstations with a basic set of components, a workstation for simple mechanical tasks, and various lab equipment such as power supplies, frequency generators, multimeters, oscilloscopes, DAQs, impedance analyzers, and de-bugging tools for embedded systems.

### Laser and THz-Photonics laboratory

In this lab spectroscopy systems for visible (UV/Vis) and invisible (THz) range are available or under further development. Using fs-laser pulses, THz beams are generated via nonlinear effects in an organic crystal, which are sent through a sample under investigation to determine its properties non-invasively. Visible spectroscopy on temperature-dependent samples is measured in a vacuum chamber. A supercontinuum laser system was acquired in 2022 with co-funding from the Swiss National Science Foundation.

### Thin film characterization laboratory

In this laboratory, various instrumentation is available to study thin film samples with angle-dependent ellipsometry, profilometry, 3D optical microscopy, FTIR spectroscopy.

### Nano-Imaging laboratory

Current research on perovskite semiconductors requires information on the nanoscale. For this purpose, an atomic force microscope (AFM) combined with an optical spectrometer was acquired in 2022. It is a highly technical complex device that allows confocal optical microscopy such as luminescence and Raman, which can be combined with AFM techniques to allow near-field measurements. The investment was paid by the ERC Grant OptElon (grant agreement no. 851676).

#### **Electroplating laboratory**

The heart of the electroplating laboratory is an experimental copper refining electrolysis cell. In this electrolysis cell, controlled experiments on flow-coupled ion transport phenomena can be carried out under high current but low voltage. Although originally developed for copper refining, the system can also be used to simulate alternative ion transfer processes (e.g. for galvanic coating methods). The system is fully electronically controlled, has a highly developed interface, a self-cleaning system and corresponding ventilation systems.

#### **Soft Materials Lab**

We have a fully equipped laboratory in which we can work with various soft materials (such as polymers, hydrogels, etc.) under safe conditions. Examples of available devices: 3D bioprinter (liquid printing), rod coater, ultrasonic cleaner, centrifuge, magnetic stirrer, hot plates, pH meter, etc. With these devices we can develop sophisticated prototypes for biomedical applications.

## **Thermal Design Lab**

Physicochemical computer models are valuable tools for developing new functional materials and industrial processes. However, their reliability and practical use depend heavily on the material data used. In addition, extensive calibrations and validations are usually necessary before use. With the Thermal Design Lab, we pursue the goal of generating as precise inputs as possible for our computer models using temperature and heat flow measurement technology in combination with thermal material data determination. The Thermal Design Lab currently includes a wide range of contact temperature sensors and thermal imaging cameras with different spectral ranges. We also use various methods to determine the thermal conductivities of liquids and solids.

#### Medizininformatiklabor

While the new medical informatics course is being set up, the laboratory will initially be used primarily for regular internships. Later, more and more experiments from project and bachelor theses will be carried out. As in the other thematic focuses, students in medical informatics and medical technology are also welcome to serve as assistants during the semester break in valuable support of the ICP research projects.

## A.9 ICP-Team

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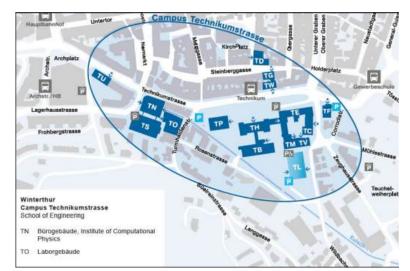
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## A.10 Location



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