

# Digitalization of Glass Development



Ulrich Fotheringham<sup>1</sup>, Leopold Talirz<sup>1</sup>, Joachim Deubener<sup>4</sup>, Tilmann Hickel<sup>2</sup>, Jan Janssen<sup>3</sup>, Ralf Müller<sup>4</sup>, Lutz Pfeifer<sup>6</sup>, Marek Sierka<sup>5</sup>, Andrea Simone Stucchi de Camargo<sup>2,5</sup>, Frederik Teepe<sup>7</sup>, Kerstin Thurow<sup>8</sup>, Moritz To Baben<sup>9</sup>, Anh Tuan Vu<sup>10</sup>, Lothar Wondraczek<sup>5</sup>

<sup>1</sup> SCHOTT AG

<sup>2</sup> BAM Bundesanstalt für Materialforschung und –prüfung

<sup>3</sup> Max-Planck-Institut für Nachhaltige Materialien GmbH

<sup>4</sup> Technische Universität Clausthal

<sup>5</sup> Friedrich-Schiller-Universität Jena

<sup>6</sup> LTB Laser Technik Berlin GmbH

<sup>7</sup> PRALL-Tec GmbH

<sup>8</sup> Universität Rostock

<sup>9</sup> GTT Technologies

<sup>10</sup> Fraunhofer-Institut für Produktionstechnologie IPT



SPONSORED BY THE



Pioneering the impossible since 1884



**1884**

Optical  
glass



The most precise  
microscopes



**1911**

FIOLAX® Borosilicate  
glass tubing



**1968**

ZERODUR®  
Glass-ceramic



The world's largest  
telescopes

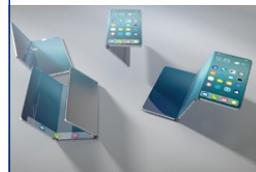


**2013**

SCHOTT UTG®  
ultra-thin glass

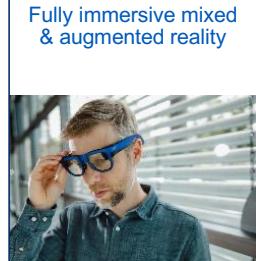


Guinness World Record  
– thinnest glass on earth



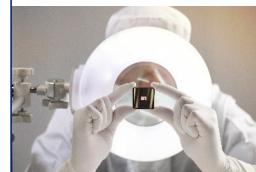
**2018**

High-index glass  
wafers & waveguides



**2024**

Glass for advanced  
chip packaging



# Vision for Specialty Glass Development and Life Cycle

**Application** determines target glass properties

## Glass Development Loop

1. **Simulation** of glass properties & process (digital twin)
2. **Robotic Melt** for automated synthesis in the lab
3. **Lab automation** for automated sample analysis

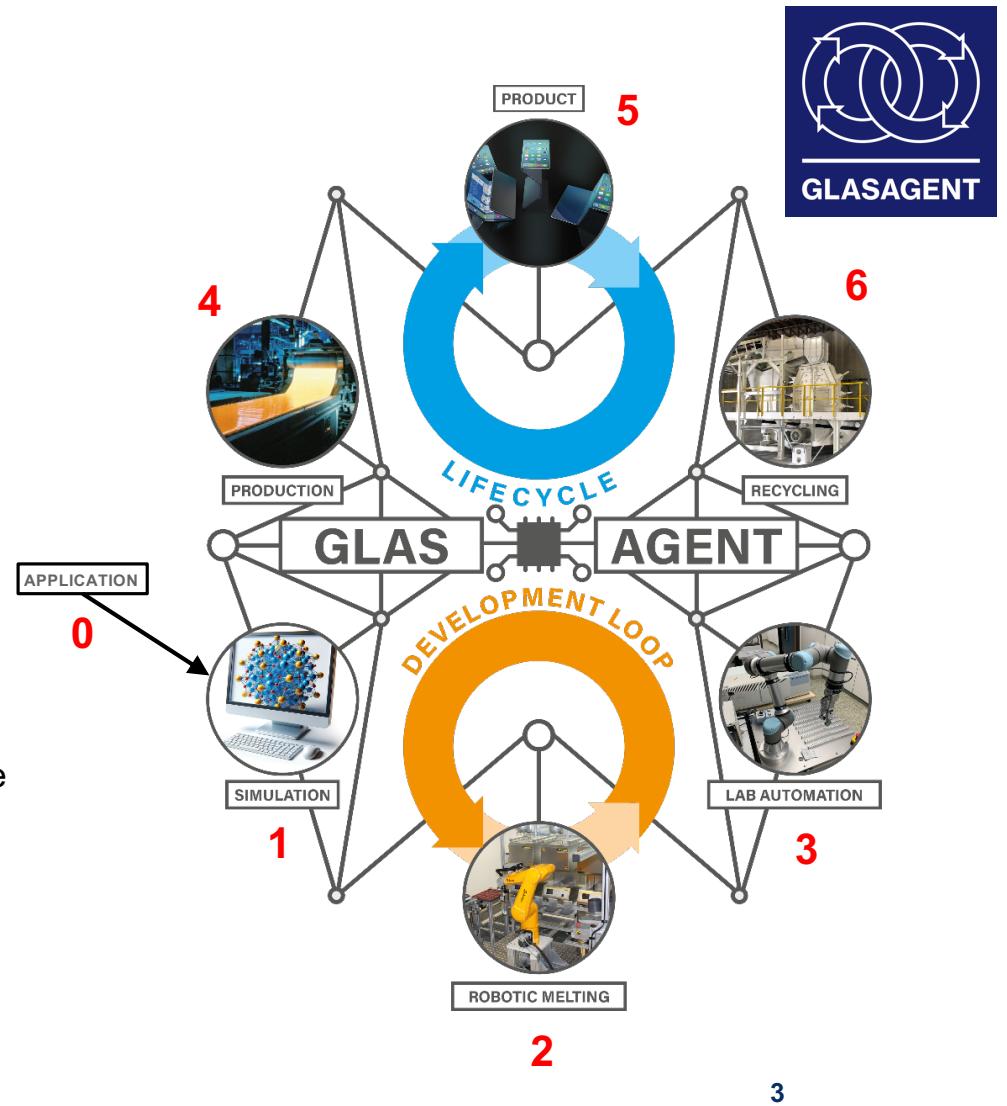
## Product Life Cycle

4. **Production** using recycled components and process parameters informed by digital twin
5. **Product use** without compromises in safety & performance
6. **Recycling** with separation of different special glass types

## Spider in the Web

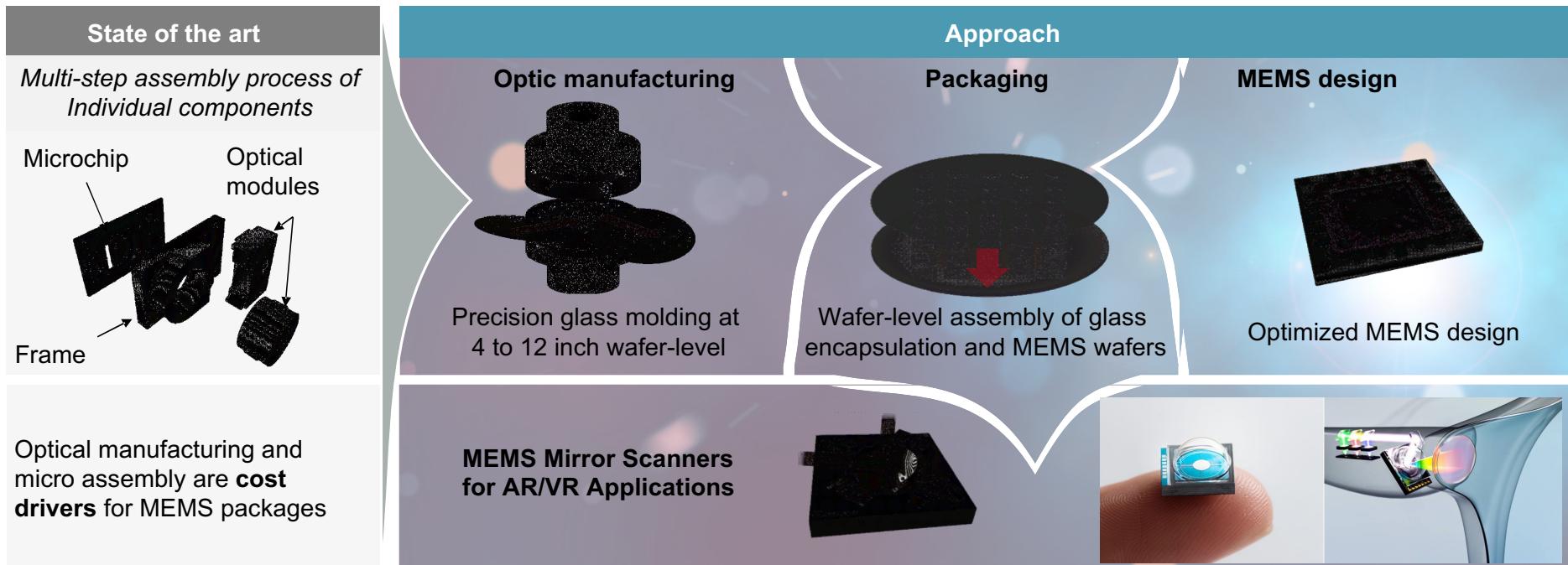
**GlasAgent**: Software agent integrating these loops

MaterialDigital 3, Project GlasAgent



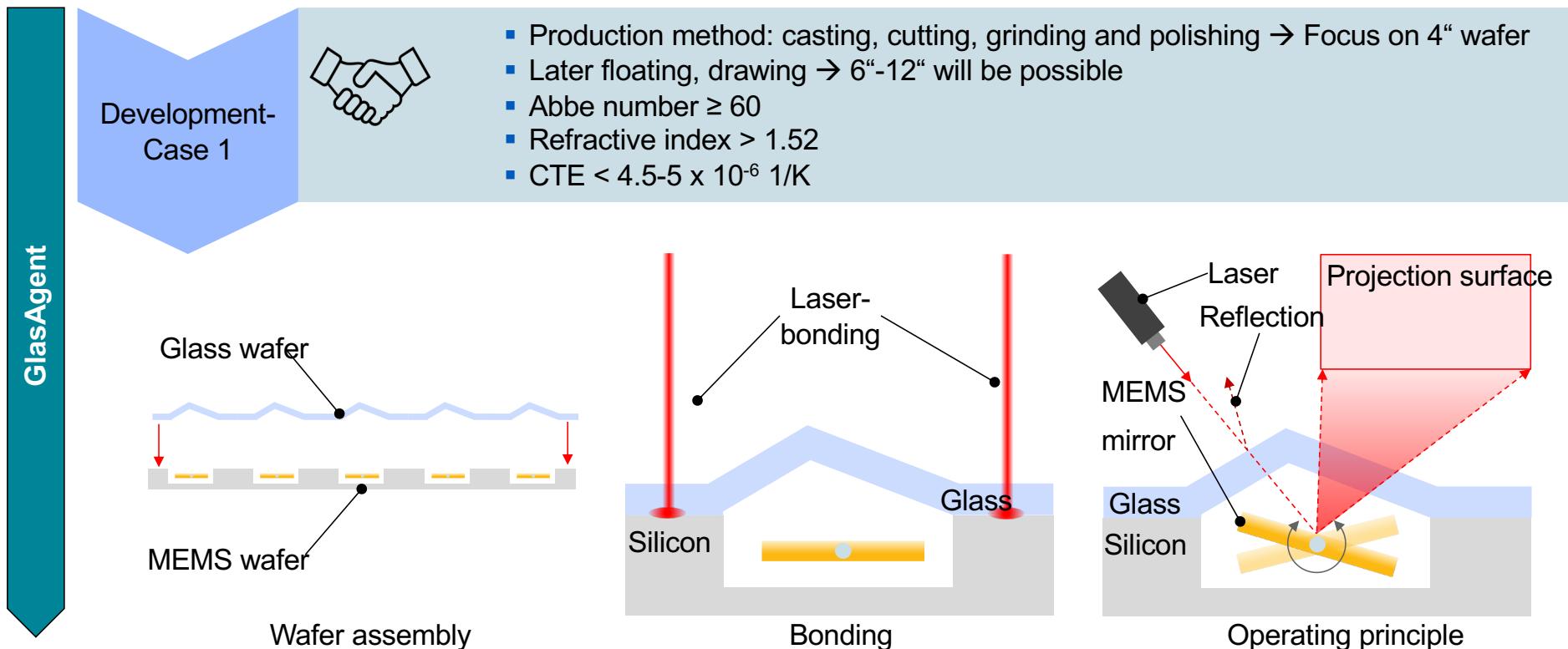
# Application

New special glass for cost-effective optoelectronic components by wafer-level precision glass molding



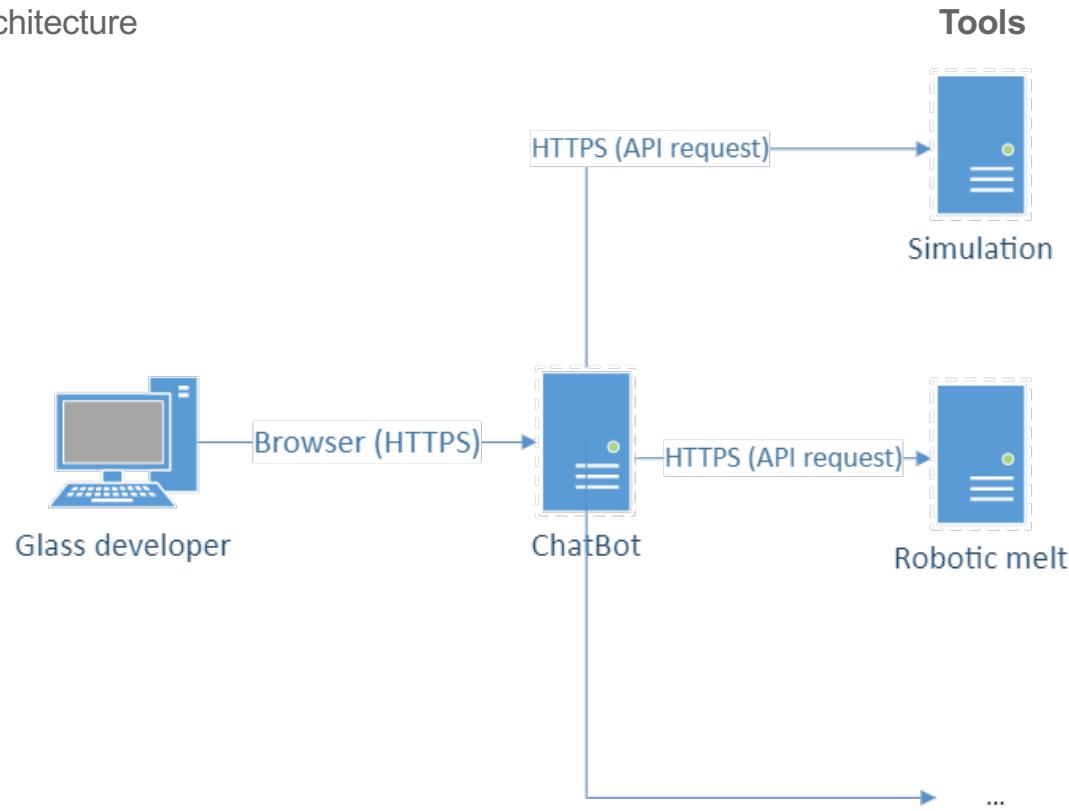
# Application

## New specialty glass for cost-effective optoelectronic components: optocaps for projector MEMS



# GlasAgent

## Architecture



### Tools

- Databases (glass properties, patents, ...)
- Models that predict glass properties based on composition
- Thermodynamic simulations via GTT
- Atomistic simulations via pyiron workflows
- Melt request for robotic melts
- ...

### Ontology

- Starting from GlasDigital ontology (MaterialDigital 1)
- Include relevant ISO and DIN standards for raw materials, processing, analysis & recycling
- Integrate description of simulation methods for digital twin

# GlasAgent

Chat Mockup

Glass Developer  
Hello Otto, I'm looking for a glass with refractive index > A,  
Abbe number > B, and CTE < C ppm/K.

► Otto searches the internal Schott database.

► Otto searches external glass database.

Otto

Unfortunately, I couldn't find any known glass with those properties. Should we try inverse design?

Glass Developer  
Yes, let's give that a try.

# Demo – SciGlass Next Search

## S SciGlass Next

- SciGlass: Open glass property database
- SciGlass Next: web interface based on SciGlass
- Add SciGlass Next MCP endpoint to your chatbot of choice!
  - Visual Studio Code
  - ChatGPT Plus (Developer Mode)
  - Claude
  - ...

The SciGlass Next interface is a web-based application designed for searching and analyzing glass properties. It features a clean, modern design with a sidebar on the left and a main content area with various panels. The panels include:

- Search Panels**: A sidebar with filters for Document, Glass, Author, and User, and a search bar for Properties.
- Data Visualization**: An interactive scatter plot showing the relationship between glass composition and properties like density or viscosity.
- Property Diagram**: A ternary diagram showing experimental property values for a selected system.
- Data Tables**: A table showing glass compositions and properties.
- Calculation Result**: A panel showing predicted properties for a specific glass composition.
- More Features**: A panel indicating that more features like commercial glass search and full-text search are coming soon.
- Optical Spectra**: A panel showing optical spectra for glasses and melts.
- Glass Formation**: A panel showing ternary diagrams of glass formation.
- Author Index**: A panel for browsing publications by author.
- Subject Index**: A panel for organizing topics.
- Property Predictor**: A panel for a Python-based ML model for predicting 85 glass properties, powered by GlassNet.

Register for free at [sciglass.uni-jena.de](http://sciglass.uni-jena.de)

# Demo – SciGlass Next Search

## S SciGlass Next

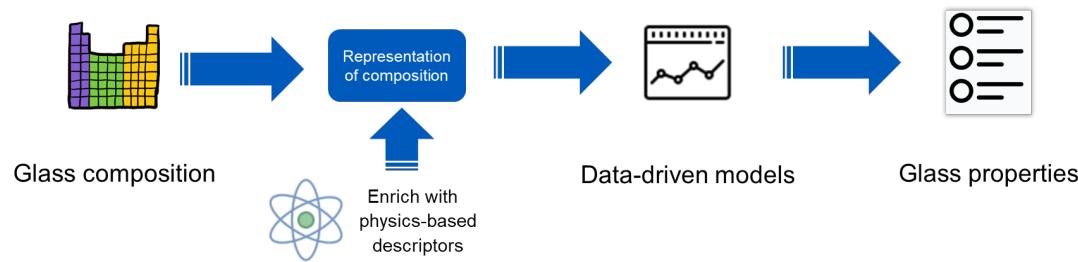
- SciGlass: Open glass property database
- SciGlass Next: web interface based on SciGlass
- Register for free at [sciglass.uni-jena.de](http://sciglass.uni-jena.de)
- Add SciGlass Next MCP endpoint to your chatbot of choice!
  - Visual Studio Code
  - ChatGPT Plus (Developer Mode)
  - Claude
  - ...
  - See SciGlass Next documentation

MaterialDigital 3, Project GlasAgent

The screenshot shows a web-based chatbot interface. At the top, there is a header with a 'Chatbot' button. Below the header, there is a large empty white area representing the message history. At the bottom, there is a message input field with the placeholder 'Message'. Inside the message input field, there is a text message: 'I'm looking for a glass with refractive index >1.52, Abbe number >60 and CTE <4.5'. To the left of the message input field is a small circular icon with a paperclip symbol. To the right of the message input field is a circular send button with a right-pointing arrow. To the right of the send button is a large grey button labeled 'Clear Chat'. In the bottom right corner of the message input field, there is a small number '9'.

# 1. Simulation

## 1.1 Data-driven models



- Given **composition** (75%  $\text{SiO}_2$ , 15%  $\text{Na}_2\text{O}$ , 10%  $\text{CaO}$ ) predict **glass properties** (glass transition temperature, ...).
- Semi-empirical and machine-learning models
- Development focus:
  - Uncertainty prediction
  - Inverse design: from property to composition

Chat Mockup

Otto  
Which material model should we use:  
1. FancyML  
2. SimpleML

Glass Developer  
Please use the FancyML model.

Otto  
All right. That will take a few minutes...

► Otto uses the FancyML model for inverse calculation. Progress [---]

Otto  
I've determined a glass composition [XYZ], with  $n=1.8$ , Abbe number 65, and CTE 4 ppm/K, but with a low confidence score. Warning: Experimental data in this property range appears to be insufficient.

Glass Developer  
That's not a bad start. What's the prediction if I increase component X by 1% and omit expensive components?

► Otto uses the FancyML model for prediction

# Demo – SciGlass Next Prediction

## S SciGlass Next

- Using GlassNet model by D. Cassar et al.

Chatbot

- $\text{CTE} = 3.9 \text{ ppm/K} (39 \times 10^{-7} \text{ K}^{-1})$
- **Composition (mol%)**:  $\text{P}_2\text{O}_5$  53.09,  $\text{SiO}_2$  29.51,  $\text{Al}_2\text{O}_3$  17.39

This glass has the **highest Abbe number** and a **low CTE**, though its refractive index is only slightly above your threshold.

If you want a higher refractive index while keeping Abbe > 60 and CTE low, the best compromise is:

**Glass No. 192520 / 192529 (2000)**

- $n_d = 1.549$
- **Abbe number** = 65.51
- $\text{CTE} = 4.49 \text{ ppm/K} (44.9 \times 10^{-7} \text{ K}^{-1})$
- **Composition (mol%)**:  $\text{CaO}$  4.36,  $\text{MgO}$  15.15,  $\text{Na}_2\text{O}$  2.96,  $\text{SiO}_2$  71.04,  $\text{ZrO}_2$  5.9,  $\text{Al}_2\text{O}_3$  0.6

Do you want me to **optimize for the absolute highest Abbe number** or for a **balanced high  $n_d$  and low CTE**?

Message

How do the properties of the last glass compare against ML predictions?

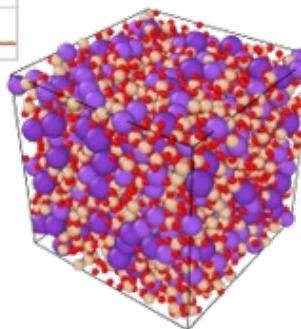
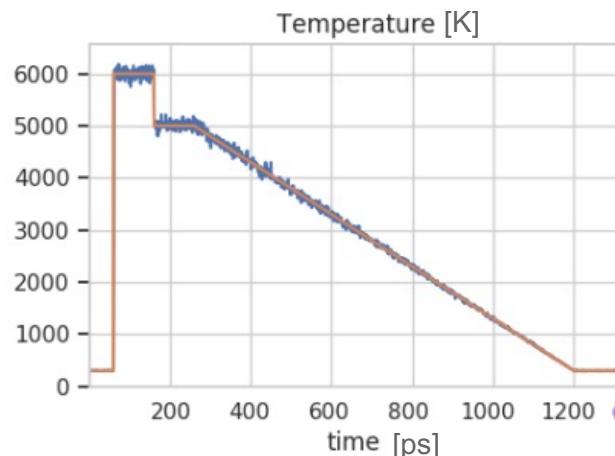
Clear Chat



# 1. Simulation

## 1.2 Atomistic simulations

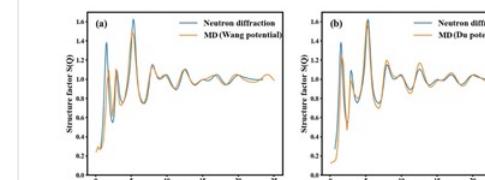
### Glass structure from melt-quench procedure



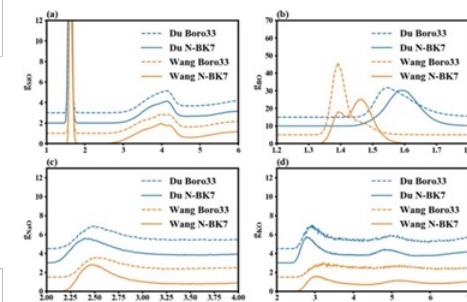
MAX PLANCK INSTITUTE  
FOR SUSTAINABLE MATERIALS

SCHOTT  
glass made of ideas

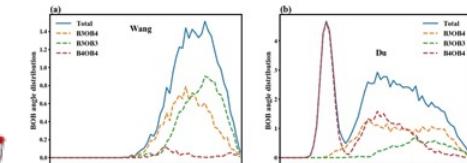
### → Properties



### Structure factors



### Radial distribution functions



### Angle distributions functions incl. projections

Condition	Boro-33	N-BK7
Experiment	2.23	2.51
Wang	2.35±0.06 (+5 %)	2.51±0.01 (+0 %)
Du	2.34±0.01 (+1.14 %)	2.48±0.01 (-0.8 %)

### Densities

Condition	Young's modulus (GPa)	Bulk modulus (GPa)	Shear modulus (GPa)	Poisson's ratio
Boro-33 (Experiment)	64	35.5	26.5	0.2
Boro-33 (Du NVT)	85.8±2.7 (+34 %)	51.3±3.5 (+42 %)	35.1±1.1 (+32 %)	0.22±0.02 (+10 %)
Boro33	51.9±3.4	29.1±1.2	21.6±1.7	0.20±0.02

### Elastic constants

12

Deng, L., and Du, J. 2018. J Am Ceram Soc 101(2):403.  
Lee, K.-H., et al. 2020. Journal of Non-Crystalline Solids 528:119736.

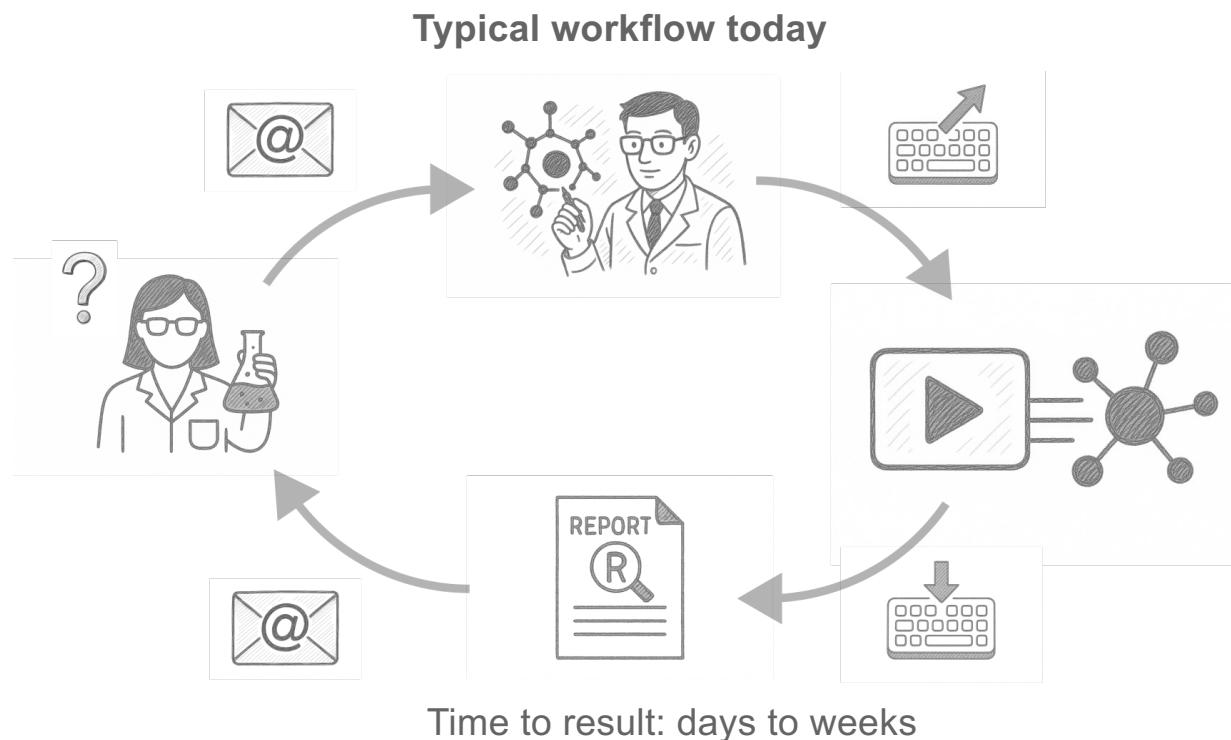
# 1. Simulation

## 1.2 Atomistic simulations



MAX PLANCK INSTITUTE  
FOR SUSTAINABLE MATERIALS

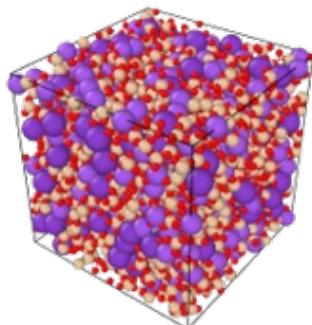
SCHOTT  
glass made of ideas



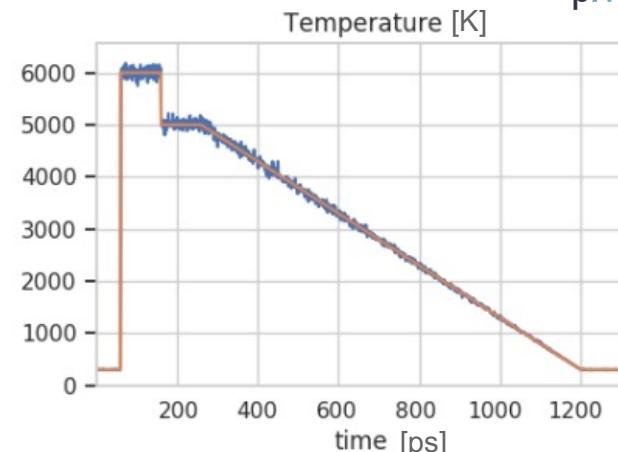
# 1. Simulation

## 1.2 Atomistic simulations

- Automated workflows for melt-quench procedure & property calculations
  - Using pyiron workflow manager
  - Targeting time to result: ~12h
- Classical & machine-learning force fields



Melt-quench workflow



MAX PLANCK INSTITUTE  
FOR SUSTAINABLE MATERIALS

SCHOTT  
glass made of ideas

### Chat Mockup

Glass Developer  
Let's start development with the following three compositions: [...].

► Otto creates order for robotic melt.

Otto  
Here are the melt orders with suggested raw materials.  
[Download/View] Submit?

Glass Developer  
That won't get done today anyway. Let's run the standard simulations overnight.

► Otto starts thermochemical melt simulations with GTT/FaCCT Sage.

► Otto starts atomistic simulations of glass composition and properties using universal ML potential. Runtime: 12 hours.

Otto  
The simulated CTE for composition 3 deviates significantly from the target.

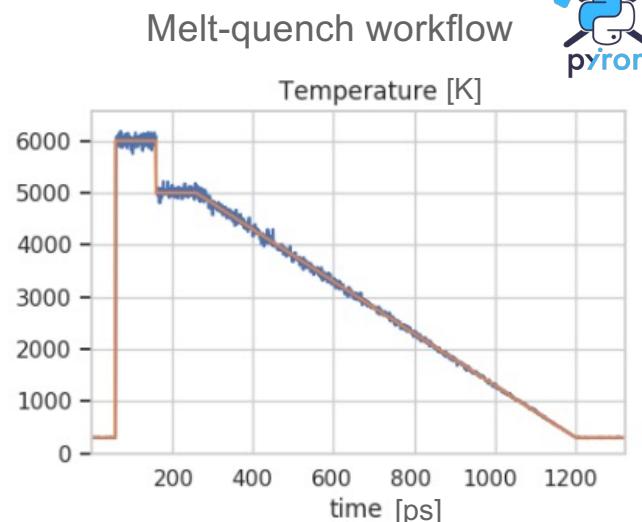
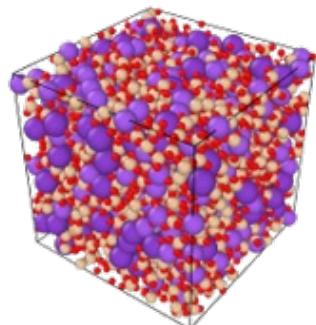
Glass Developer  
Please submit the melt order for the other two compositions.

► Otto sends order to robotic melting facility.

# 1. Simulation

## 1.2 Atomistic simulations

- Automated workflows for melt-quench procedure & property calculations
  - Using pyiron workflow manager
  - Targeting time to result: ~12h
- Classical & machine-learning force fields



MaterialDigital 3, Project GlasAgent



MAX PLANCK INSTITUTE  
FOR SUSTAINABLE MATERIALS

SCHOTT  
glass made of ideas

### Current work status

1. Workflow generation for:
  - Meltquench ✓
  - Viscosity ✓
  - Coefficient of thermal expansion ✘
  - Elastic moduli ✘
2. Structure analysis:
  - Radial distribution function ✓
  - Coordination numbers ✓
  - Bond angle distribution ✓
  - $Q^n$  and Network connectivity (NMR-consistent structural metrics) ✓
  - Rings ✓
3. Classical potentials ✓
4. Development of ML potential ✘

Plan to open-source classical potential workflows by April 2026 (& register them in PMD workflow store) 15

# Demo – Atomistic simulation

- Using pyiron workflow manager
- Classical force field (PMMCS)

Chatbot

Property	Original Prediction	+5% Al <sub>2</sub> O <sub>3</sub> Prediction	Change
Refractive index (n <sub>d</sub> )	1.547	1.543	-0.004
Abbe number	53.32	55.27	+1.95
CTE (ppm/K)	4.19	4.20	≈0

Interpretation:

- Increasing Al<sub>2</sub>O<sub>3</sub> slightly **lowers** refractive index but **improves** Abbe number.
- CTE remains essentially unchanged.
- The model also predicts a small increase in Young's modulus and thermal shock resistance.

Do you want me to explore whether **further** Al<sub>2</sub>O<sub>3</sub> increases could push the Abbe number above your target of 60 while keeping CTE low?

Message

I am interested in the atomic structure of this glass. Can you calculate it for me?

Clear Chat

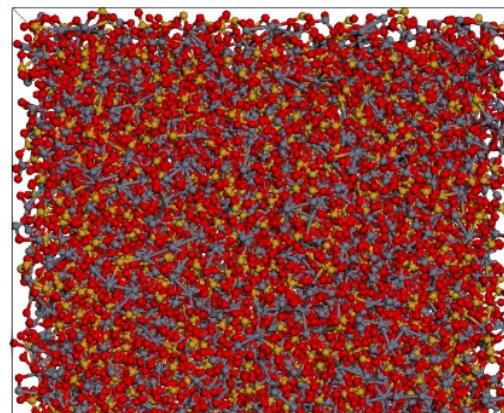
# Melt-Quench Simulation Results

Task ID: 50c135d3-8ffb-4822-ab54-f29bf0ed6aeb

Composition: 0.25CaO-0.25Al<sub>2</sub>O<sub>3</sub>-0.5SiO<sub>2</sub>

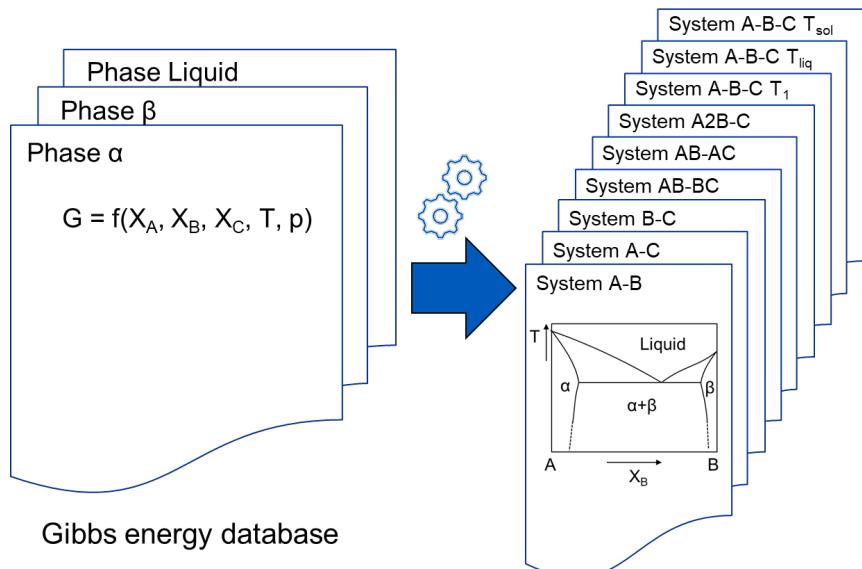
## Atomic Structure

Style: Ball & Stick Reset View



# 1. Simulation

## 1.3 Thermochemical simulations (Calphad)



### Calphad = Calculation of Phase Diagrams

- Based on GTT's GTOx database & ChemApp software
- Current development focus:
  - Expansion of thermochemical database
  - Cloud-based software solution

### Chat Mockup

Glass Developer  
Let's start development with the following three compositions: [...].

► Otto creates order for robotic melt.

Otto  
Here are the melt orders with suggested raw materials.  
[Download/View] Submit?

Glass Developer  
That won't get done today anyway. Let's run the standard simulations overnight.

► Otto starts thermochemical melt simulations with GTT/FaCCT Sage.

► Otto starts atomistic simulations of glass composition and properties using universal ML potential. Runtime: 12 hours.

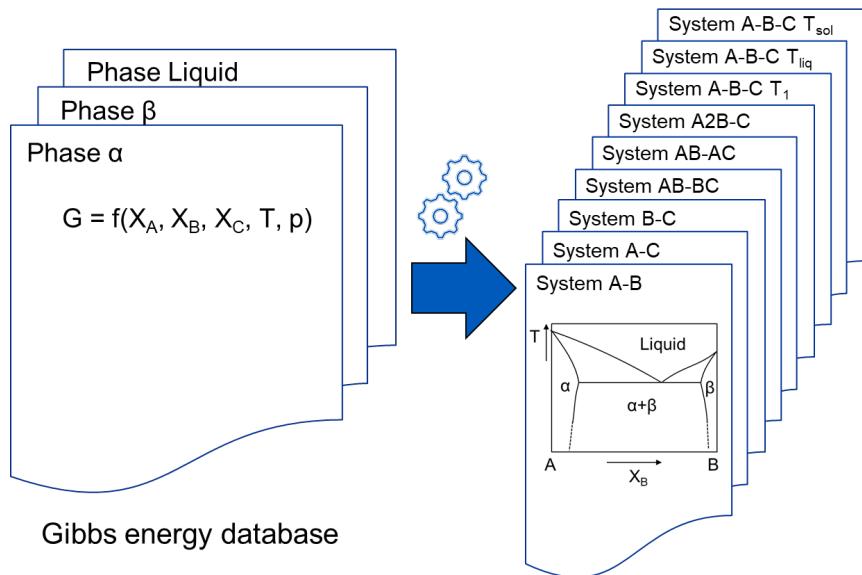
Otto  
The simulated CTE for composition 3 deviates significantly from the target.

Glass Developer  
Please submit the melt order for the other two compositions.

► Otto sends order to robotic melting facility.

# 1. Simulation

## 1.3 Thermochemical simulations (Calphad): overview and current work



### Calphad = Calculation of Phase Diagrams

- Based on GTT's GTOx database & ChemApp software
- Current development focus:
  - Expansion of thermochemical database
  - Cloud-based software solution

### Current work status

- Beta version of GTOx with B2O3 circulated
- Experiments on enthalpy of mixing ongoing at Schott
- Internal demo of cloud-based CalPhaD optimizer
- Prototype integration with GlasAgent

# Demo – ChemSage liquidus line

- Using GTT ChemApp
- Feature: predict liquidus temperature along a one-dimensional composition range

Chatbot

- CaO solid
- $\text{CaCO}_3$
- $\text{CaSiO}_3$  polymorphs: wollastonite, pseudowollastonite
- $\text{Ca}_2\text{SiO}_4$  polymorphs: olivine  $\gamma$ ,  $\alpha'$ ,  $\alpha$ , larnite ( $\beta$ )
- $\text{Ca}_3\text{SiO}_5$  (hatrurite)
- $\text{Ca}_5\text{Si}_2\text{O}_7$  (rankinite)

We can now:

- Run **equilibrium calculations** for any mixture of these components.
- Calculate **liquidus temperatures** along a composition axis.
- Explore **phase stability** over temperature/pressure ranges.

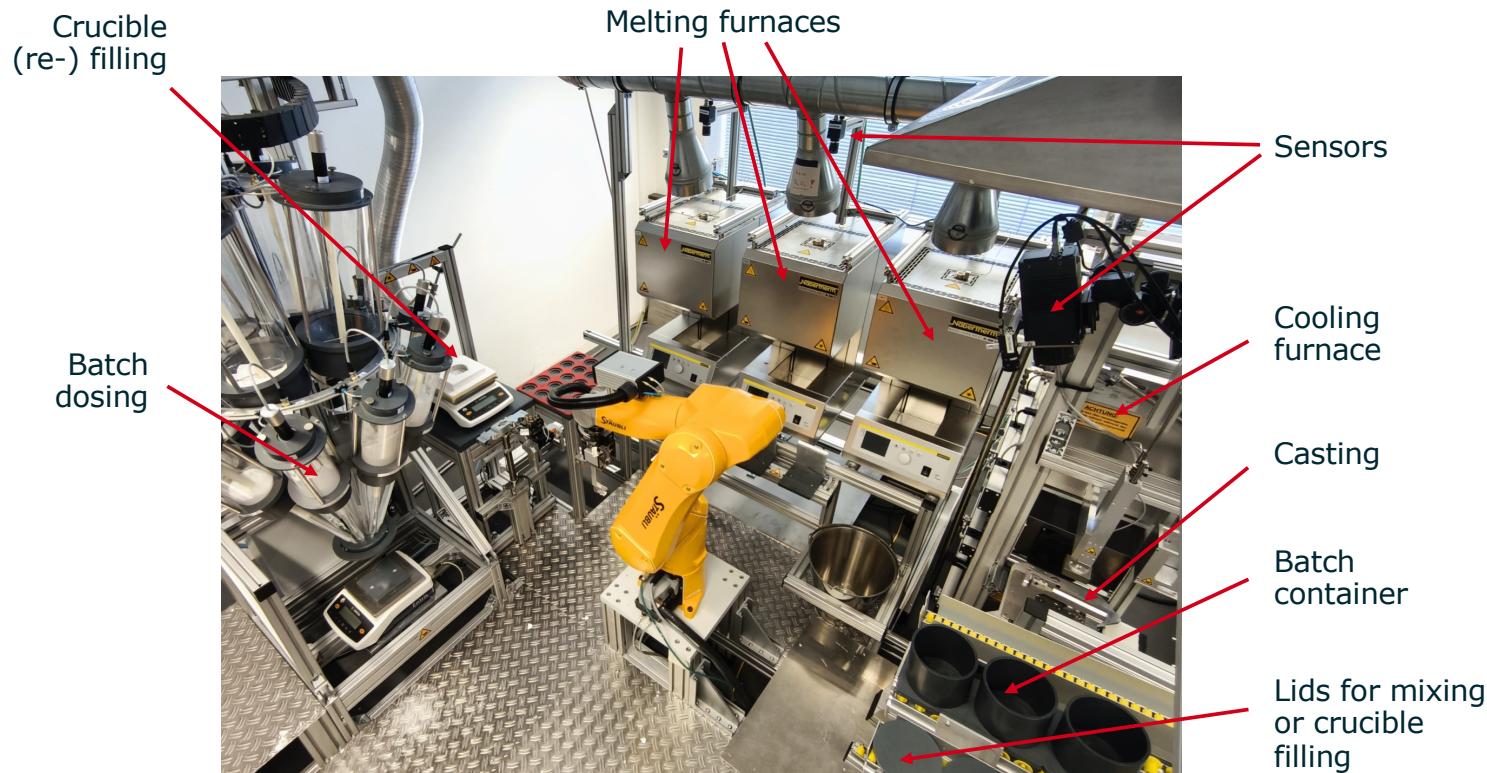
Do you want me to demonstrate an **equilibrium calculation** for a specific oxide mixture?

Message

Let's start with a liquidus line. Show me how the liquidus temperature changes, going from silica to a typical soda-lime glass.

Clear Chat

## 2. Robotic Melting System: overview



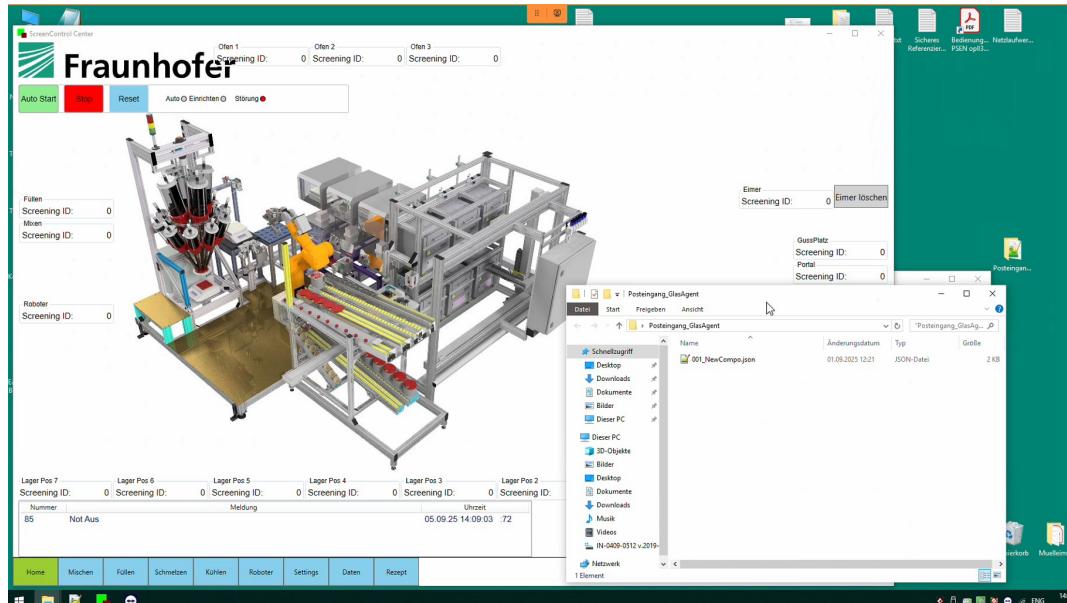
**Goal: Step by step optimization**

1. Automated definition of process parameters in the control software
2. Inline homogenization and measurement of viscosity & density

## 2. Robotic Melting System: current work

**Implementation of automated definition of process parameters in the control software**

**First milestone:**  
 GlasAgent may electronically communicate melting orders to robotic melting system

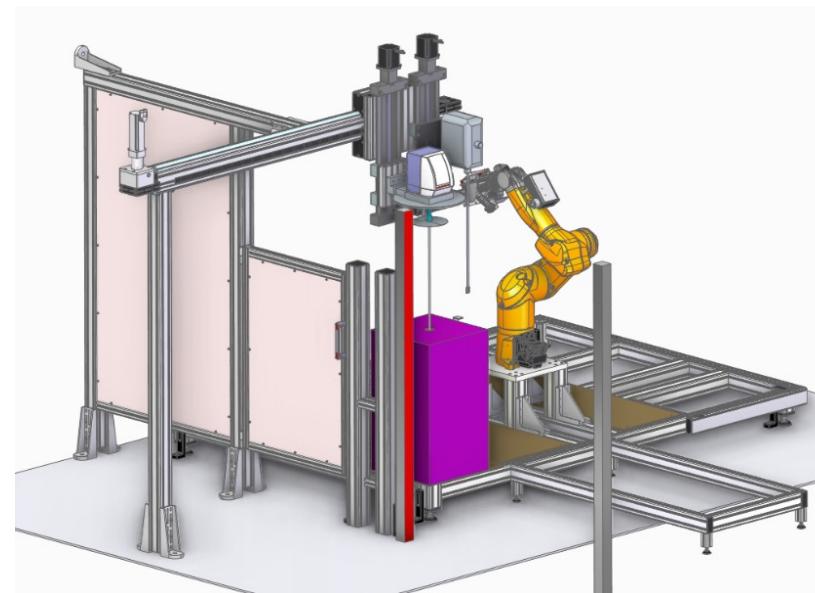


## 2. Robotic Melting System: current work (continued)

### Inline Viscosity

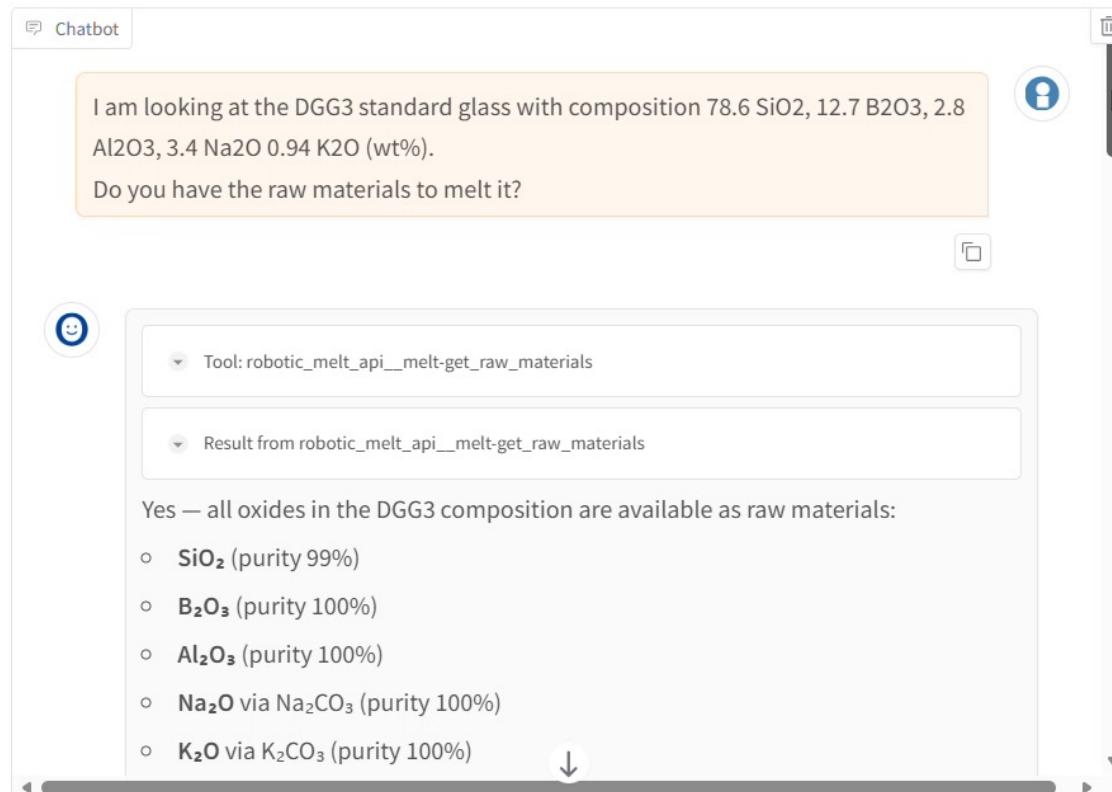
- Construction of an **induction furnace**
- with **stirring unit** for homogenizing the melt and
- a **rheometer measuring head** for adjusting the viscosity before casting

➤ Improvement of reproducibility and quality of glass blocks



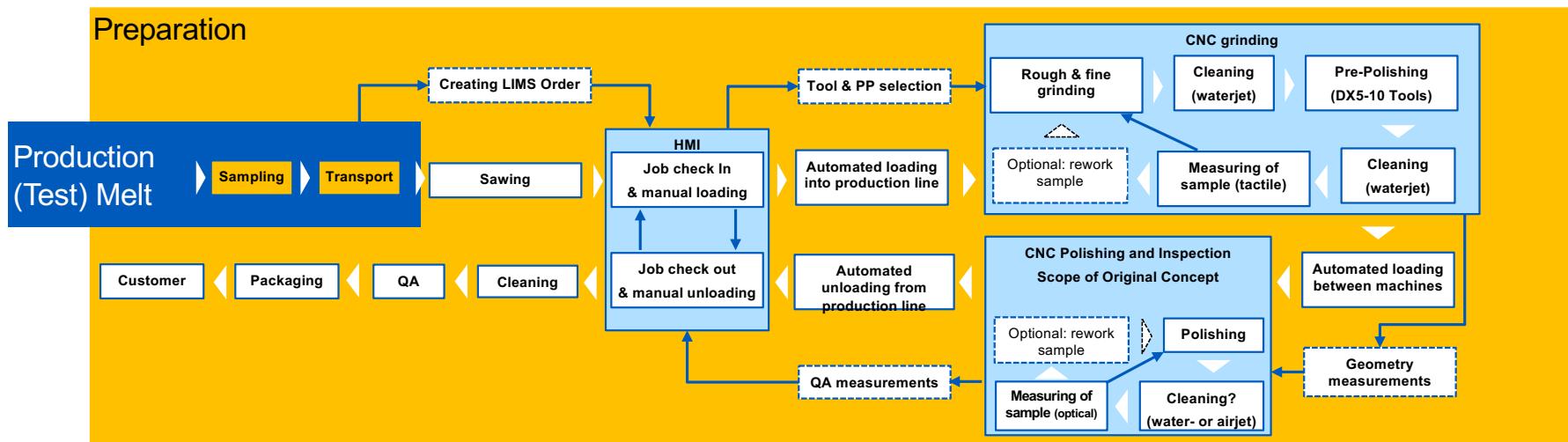
## Demo – Submit melt request

- Using robotic melt API



### 3. Automated Lab: bottleneck #1 sample polishing

#### 3.1. Outline of a fully automated system



**Goals:**

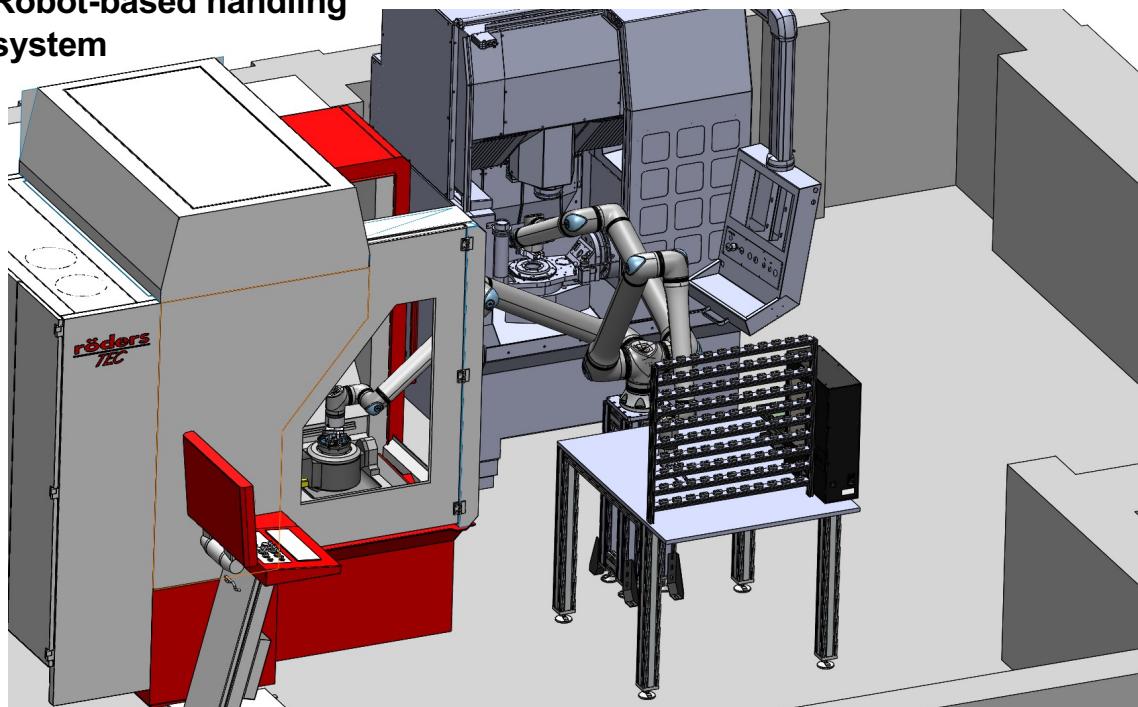
1. **Automated sample preparation for glass analysis: optical properties, chemical resistivity, mechanical strength, thermal properties; process time reduced to hours**
2. **Required(1): robot-based handling system**
3. **Required(2): camera-based automated quality control system for polishing processes**

PP: Process Parameter  
 Material flow  
 Information flow

## 3. Automated Lab: bottleneck #1

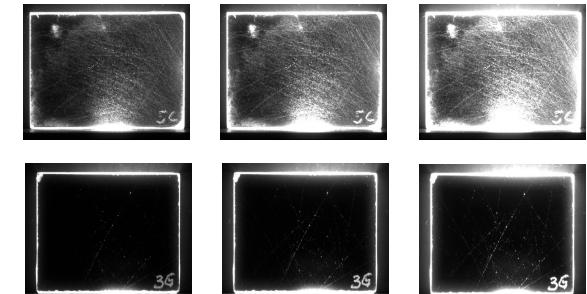
### 3.2 Some pictures

Robot-based handling system



Camera-based automated quality control system for polishing processes:

At which stage is the scattering at the surface so small that polishing is finished?



### 3. Automated Lab: bottleneck #2 wet chemistry

#### 3.1 Idea: LIBS for quantitative glass analysis

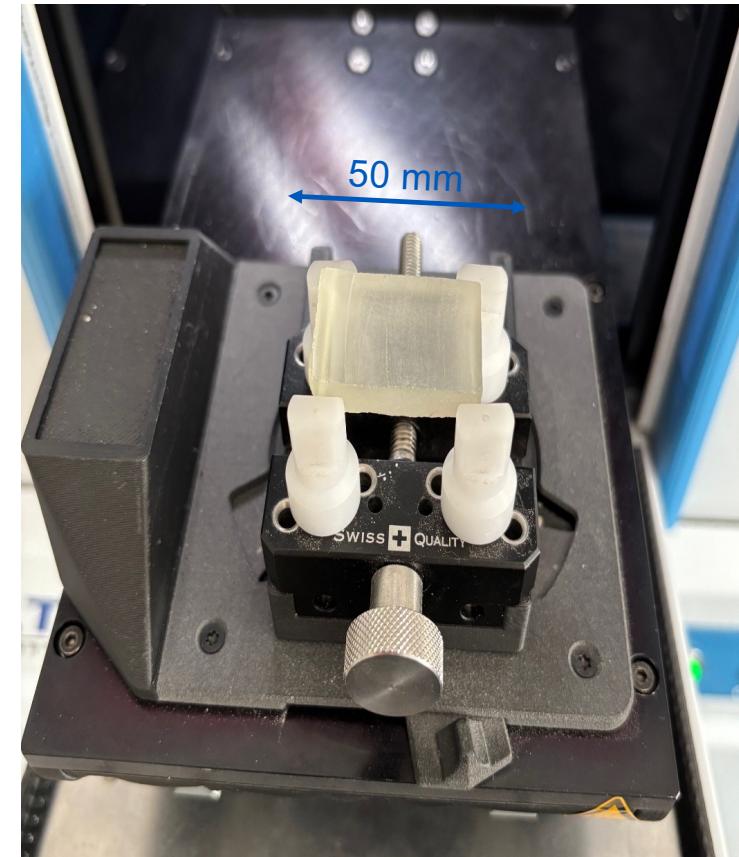
LIBS = Laser-Induced Breakdown Spectroscopy

##### Working Principle

1. Laser-Induced ablation, creating  $\mu\text{m}$ - to mm-size plasma
2. Optical emission spectroscopy of the plasma
3. Concentration of elements derived from intensity of characteristic spectral lines.

##### Goal

1. Feasibility of quantitative glass analysis
2. Replacement of wet chemistry



### 3. Automated Lab: bottleneck #2

#### 3.2 Status of: LIBS for quantitative glass analysis

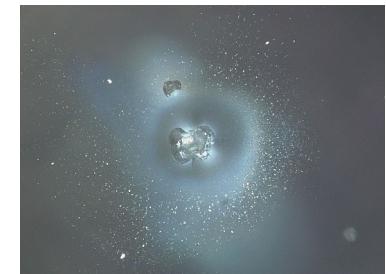
- LIBSpector arrived at BAM and under implementation
  - Integration in the robotic melting system necessary
- Oven for LIBS on melted glass is set-up in the LTB laboratory
  - New design of OEM-LIBS necessary



- First CAS glass calibration measurements with LIBSpector at BAM:
  - Repeat validation at the new location
  - Test for new CAS glass melts (CAS: Ca-Al-Si)
- Calibration on Borosilicate glasses was tested and laser parameters have to be changed to ensure similar impact on different glasses



undesired impact

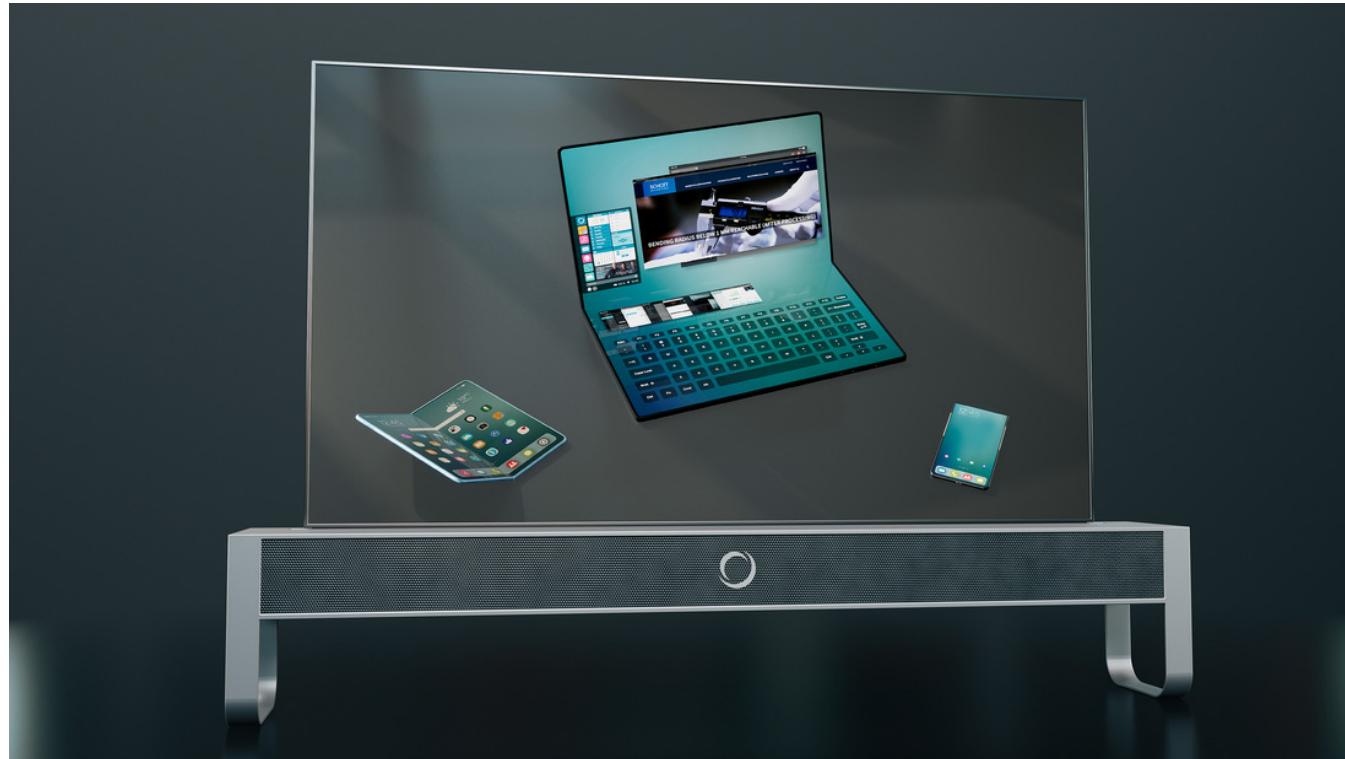


desired impact

## 4. Production



## 5. Product use at customer



## 6. Recycling

### 6.1. Separation of components from complex devices

- Innovative company specializing in various recycling technologies
- Broad product portfolio:  
Impact Crushers, Hammer Mills, Shredders, Screening and Sorting Systems

#### Areas of Application:



**SOLAR**



**LAMINATED GLASS**

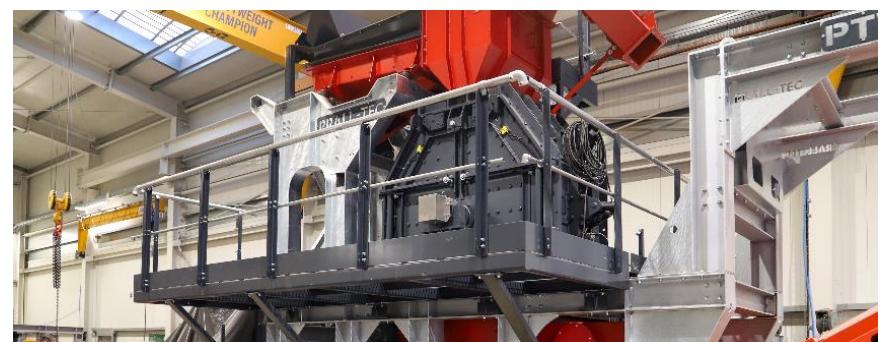
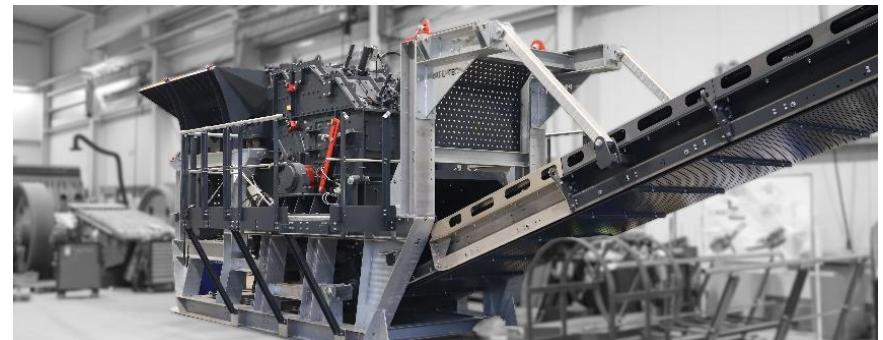


**FLOAT GLASS**



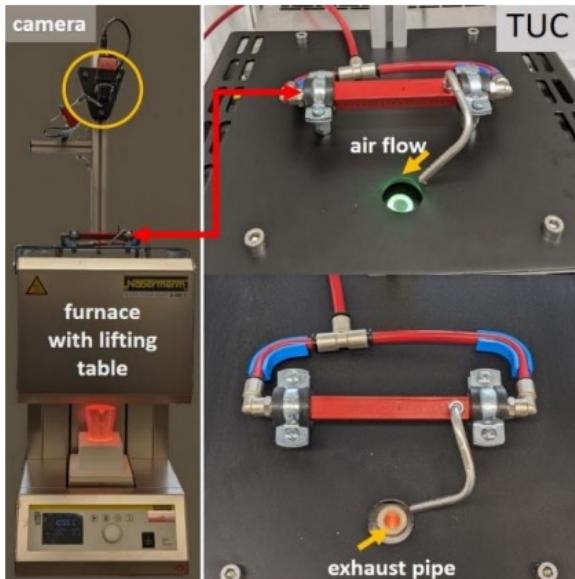
**E-SCRAP**

#### Plant Engineering:

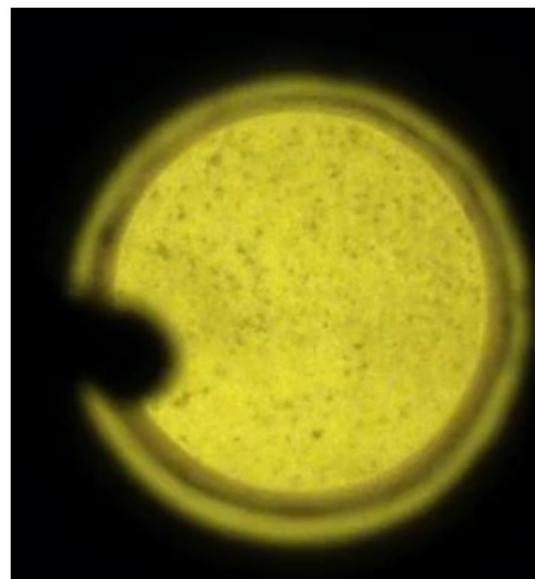


## 6. Recycling

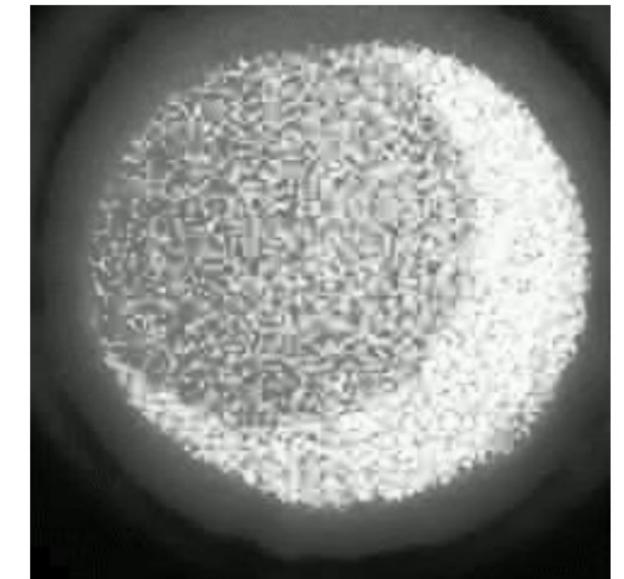
### 6.2. Test of melting behaviour



Electrical furnace with a **camera**  
Monitoring through a narrow  
 $\text{Al}_2\text{O}_3$  tube



**ML- Image analysis**  
Melt stages (ResNet34)  
Granules → Foaming → Fining



**ML- Image analysis**  
Castability check (Mechanical impact →  
Image change rate reflects viscosity)\*

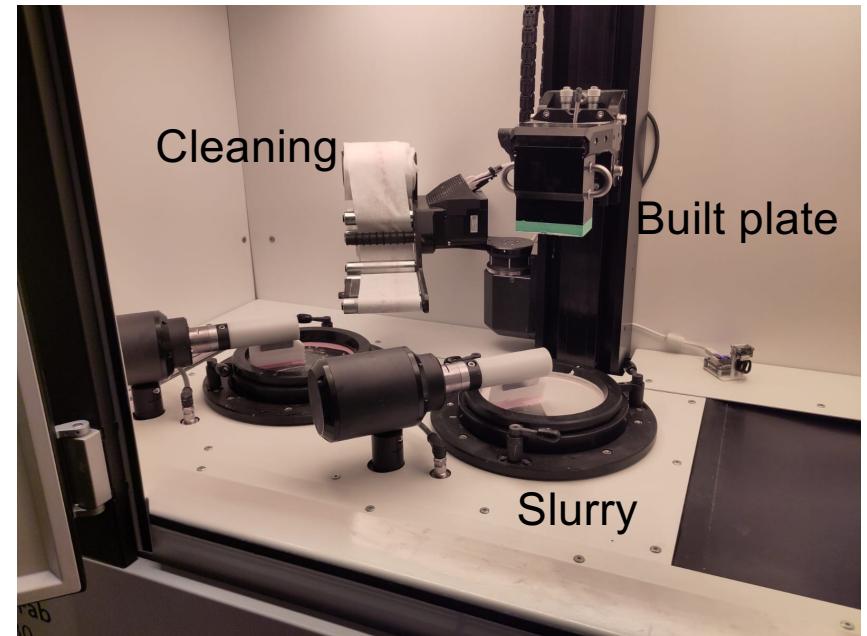
## 6. Recycling

### 6.3. High-Throughput Glass Characterization

3D printer



Multi-component printing



## 6. Recycling

### 6.3. High-Throughput Glass Characterization

First step is a 3D-print of a suitable slurry consisting of glass precursors and organics

Second, organics get burned off and glasses with different compositions remain

Next step is upscaling the process to the desired sample amount

Current working is on ways of characterizing the quality and reliability of the print



# GlasAgent

- **Goal 1:** accelerate specialty glass development through
  - Easy-to-use digital tools via chatbot interface
  - Automatic simulation workflows
  - Robotic melting system
  - Sample preparation for any analysis by automated polishing
  - LIBS for fast composition measurement
  - Demonstrator: development of special glass for optoelectronics
- **Goal 2:** enable recycling of special glasses & integrate it into the development process
- **Partners:** 10 partners from industry, university & research institutes with leading expertise
- **Duration:** 01/2025 - 12/2029

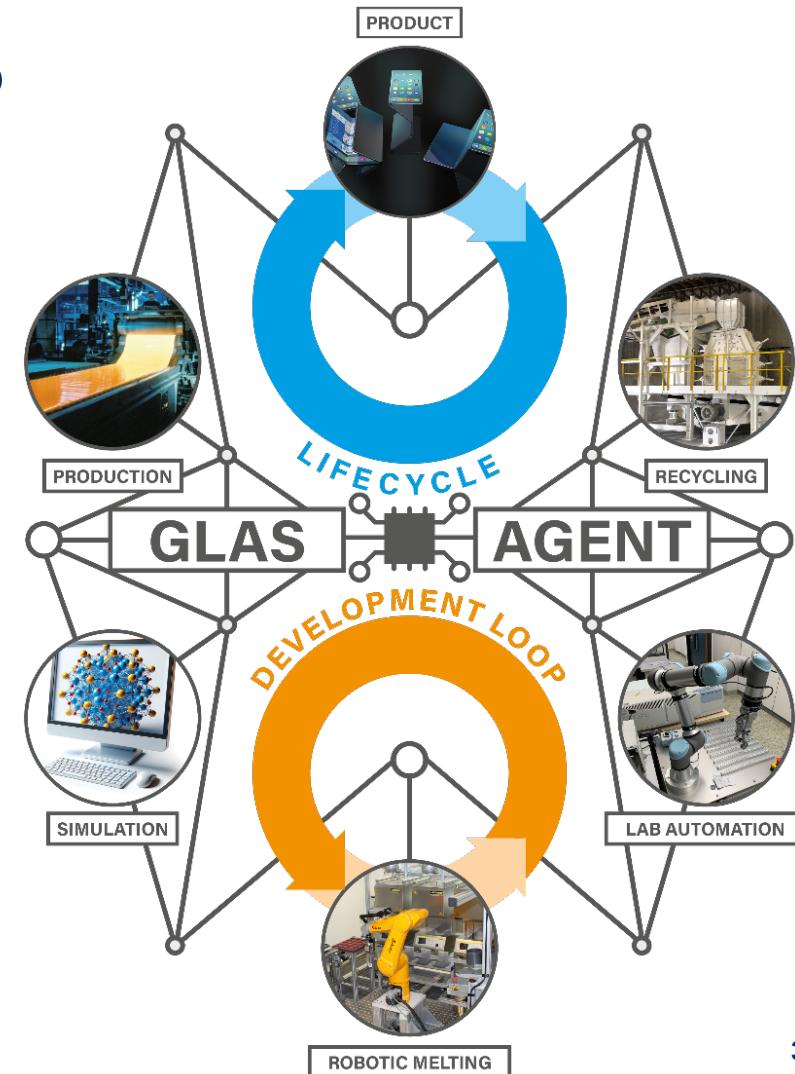
SPONSORED BY THE



# GlasAgent says “Thank you” to

- Achraf Atila, BAM
- Stefan Reinsch, BAM
- Tina Waurischk, BAM
- Heiko Engelhardt, CELISCA (U Rostock)
- Igor Seibel-Geraschenko, FSU Jena
- Ya-Fan Chen, FSU Jena
- Florian Tang, GTT
- Alexander Walnsch, GTT
- Albina Karimova, IPT
- Steffen Mittelmann, LTB
- Kai Richter, PRALL-Tec
- Bastian Barwick, SCHOTT
- Detlef Köpsel, SCHOTT
- Marcel Sadowsky, SCHOTT
- Enzo Henrique Miguel, TUC

SPONSORED BY THE



# Discussion

