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in chemical space.

**GTT-Technologies**

# USERS' MEETING 2026



[www.gtt-technologies.de](http://www.gtt-technologies.de)

## Wednesday Afternoon (July 8)

13:00 *Arrival & Coffee*

### From Earth to Moon

14:00 Welcome & Introduction

Moritz to Baben, Stephan Petersen, Philipp Keuter (GTT-Technologies)

14:20 Application of Thermodynamic Modeling with FactSage in Steelmaking  
Olena Volkova (TU Bergakademie Freiberg) 


15:00 Thermodynamic Modeling and Experimental Validation of Metallurgical Processes Using FactSage  
Bora Derin (Istanbul Technical University)

15:20 Modeling Hot Corrosion Induced by Aluminosilicate Deposits Found in Aircraft Turbines and Experimental Validation  
Lourdes Camarma (Forschungszentrum Jülich)

15:40 Application of Thermodynamic Calculation to Oxygen Extraction from Lunar Minerals under Vacuum Conditions  
Masanori Suzuki (Kindai University)

16:00 *Break*

### Future Under Construction

16:20 Use of FactSage and related tools in building materials research  
Alexander Pisch (CNRS Grenoble) 

16:50 Development of new carbonatable clinker compositions  
Arne Peys (VITO)


17:10 KilnSimu – Beyond Equilibrium  
Shivani Gonde, Cassie Früh (GTT-Technologies)

17:30 *End of day*

## Thursday Morning (July 9)

08:40 *Morning Coffee*

### Full Circle

09:00 A Thermodynamic Understanding of the Opportunities and Limits of the Circular Economy  
Markus A. Reuter (ElvalHalcor, TU Freiberg, Stellenbosch University) 

09:45 Why Predictive Modeling of Materials and Processes Is So Difficult  
Moritz to Baben (GTT-Technologies)

10:15 *Break*

10:30 Synergistic Valorization of Waelz, Linz-Donawitz, and Fayalite Slags  
Junnile Romero (Helmholtz HIF) 

10:50 MD-informed structure-property model for self-diffusion coefficients in CaO-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> slags  
Hélène Verbeeck (UGent)

## Beyond Equilibrium

- 11:10 How to accurately model the DRI metallization degree?  
Anna Ravensburg (GTT-Technologies)
- 11:35 Agentic Coding in ChemApp for Python  
Bruno Reis (GTT-Technologies)
- 12:20 *Lunchbreak*



## Thursday Afternoon (July 9)

- 13:30 *Constraints I: What Are Constraints in Thermodynamics and Where Do They Come From in Reality?*  
Moritz to Baben (GTT-Technologies)
- 13:45 *Constraints II: GTOx for Glasses – Kinetic Limitations Between Condensed Phases*  
Philipp Keuter (GTT-Technologies)
- 14:05 *Constraints III: Kinetic limitations in the Gas Phase – Understanding Methanol Synthesis*  
Anna Ravensburg (GTT-Technologies)
- 14:20 *Constraints IV: Electrolysis Driving Kinetics Beyond Unconstrained Equilibrium – The Hall-Heroult Process*  
João Rezende (GTT-Technologies)
- 14:40 *Constraints V: Explicit Treatment of Microstructural Defects – Partitioning at and Energy of Grain Boundaries*  
Moritz to Baben (GTT-Technologies)
- 15:00 *Break*



## Beyond the Database

- 15:20 Database Development for InP Synthesis and Crystal Growth  
Marius Wetzel (Fraunhofer IISB)
- 15:40 Molar Volume Prediction of Liquid Alloys Using Modified Quasichemical Model  
Min-Kyu Paek (TU Clausthal)
- 16:00 Calphad Optimizer 3.1: Building Interoperable Workflows  
Florian Tang (GTT-Technologies)

## Breakout Sessions: Developer Exchange

- |   |                                    |
|---|------------------------------------|
| 16:30 Predictive Modeling of Materials and Processes<br>Moritz to Baben | Database Selection<br>João Rezende |
| Getting Started with Agentic Coding<br>Fabrice Yang, Ömer Büyükuslu     | KilnSimu<br>Shivani Gonde          |
| ChemApp for Python<br>Bruno Reis  | Calphad Optimizer<br>Florian Tang  |
- + *Networking & Refreshments*



18:00 *End of day*





19:30 *Group Dinner: L'Osteria Kapuzinergraben, Kapuzinergraben 19, 52062 Aachen*



## ● Friday Morning (July 10)

### ● The Digital Process Toolbox

- 08:40 *Morning Coffee* 
- 09:00 Simplified Process Modeling for Copper Metallurgy Using FactSage and ChemApp for Python  
Shivani Gonde (GTT-Technologies)
- 09:30 FactFlow: A New FactSage Tool to Simulate Pyrometallurgical Processes – Application for Ferro-Niobium Production  
Jean-Philippe Harvey (ThermFact / CRCT)
- 10:00 ChemApp for SysCAD – Plant-Wide Flowsheet Simulation: Seven Years of Experience  
Tanai Marin-Alvarado (SysCAD)
- 10:20 *Break* 
- 10:40 Gasifier Feed-Forward Control by Means of Thermodynamic Modeling of the Slag Behavior  
Johan van Dyk (GTI Energy)
- 11:00 High-Throughput Materials Informatics Integrating *ab initio*, Machine Learning and CALPHAD Data  
Irina Roslyakova (GTT-Technologies)
- 11:20 User Experience Design for Equilib2.0  
Moritz to Baben (GTT-Technologies)
- 11:50 Farewell

## ● Info

- Venue [Forum M](#)  
[Buchkremerstraße 1-7, 52062 Aachen](#)
- Group Dinner [L'Osteria Kapuzinergraben](#)  
July 9, 19:30 CEST [Kapuzinergraben 19, 52062 Aachen](#)
- Website Find the **abstracts** and all **on-site info**: [Users' Meeting website](#)

