

# 2023 Materials Design Users' Group Meeting

Austria Trend Parkhotel Schönbrunn  
Vienna, Austria, 9 –11 October 2023

## Monday, 9 October 2023

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6:00 - 8:45	Breakfast	<i>Restaurant Maria Theresia (ground floor)</i>
8:30 - 17:15	Registration & Welcome Table	Foyer near <i>Ballroom (ground floor)</i>
9:00 - 17:00	Training Sessions	<i>Franz Josef I (downstairs)</i>
10:30 - 11:00	Coffee Break	<i>Elisabeth Salon (downstairs)</i>
12:30 - 13:30	Lunch Break	<i>Restaurant Maria Theresia (ground floor)</i>
15:30 - 16:00	Coffee Break	<i>Elisabeth Salon (downstairs)</i>
<b>18:30 - 21:00</b>	<b>Welcome Cocktail Reception and Poster Session</b>	<i>Kaiserlounge (ground floor)</i>

## Tuesday, 10 October 2023

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6:00 - 9:00	Breakfast	<i>Restaurant Maria Theresia (ground floor)</i>
9:00 - 17:15	Registration & Welcome Table	Foyer near <i>Ballroom (ground floor)</i>
9:00 - 17:15	Scientific Program	<i>Ballroom (ground floor)</i>
10:35 – 11:00	Coffee Break	<i>Kaiserlounge (ground floor)</i>
11:45 – 13:45	Official 2023 UGM Group Photo Lunch	Meet in <i>Ballroom</i> <i>Restaurant Maria Theresia (ground floor)</i>
15:15 - 15:45	Coffee Break	<i>Kaiserlounge (ground floor)</i>

17:35 Please assemble near front desk for journey to venue with MD guides  
Venue address: Weitsicht Cobenzl, Am Cobenzl 94, 1190 Wien  
<https://weitsichtcobenzl.at/en/>

17:45 DEPART TOGETHER – RETURN TOGETHER

**18:15 - 22:00**                      **Annual Customer Banquet**                      *Weitsicht Cobenzl (bus with MD guides)*

## Wednesday, 11 October 2023

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6:00 - 9:00	Breakfast	<i>Restaurant Maria Theresia (ground floor)</i>
9:00 - 12:15	Scientific Program	<i>Ballroom (ground floor)</i>
14:00 – 16:00	Informal discussions between MD and Customer	<i>Ballroom (ground floor)</i>
10:15 - 10:30	Coffee Break	<i>Kaiserlounge (ground floor)</i>
12:15 - 14:00	Lunch	<i>Restaurant Maria Theresia (ground floor)</i>
15:30 - 16:00	Coffee Break	<i>Kaiserlounge (ground floor)</i>

## Thursday, 12 October 2023

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6:00 - 9:00	Breakfast	<i>Restaurant Maria Theresia (ground floor)</i>
Before 11 am	Check-out	

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## Scientific Program

Tuesday, 10 October 2023 All Technical Sessions – Ballroom (ground floor)

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6:00 - 9:00	<b>Breakfast</b>	<i>Restaurant Maria Theresia (ground floor)</i>
9:00 – 9:05	<b>Erich Wimmer</b> , Introductory Remarks and Session Chair	
9:05 – 9:50	<b>Michele Parrinello</b> , Istituto Italiano di Tecnologia, Genoa, Italy The Solid State Physics of Catalysis	
9:50 – 10:35	<b>Saad Fahaid Khalaf Al-Afnan</b> , King Fahd University of Petroleum & Minerals, Dhahran, Saudi Arabia Molecular Simulation of Natural Gas Transport in the Nano-Organic Matter of Subsurface Reservoirs	
10:35 – 11:00	<b>Coffee Break</b>	<i>Kaiserlounge (ground floor)</i>
<i>Session Chair: Volker Eyert</i> 11:00 – 11:45	<b>Georg Kresse</b> , University of Vienna, Austria Machine learning and Beyond DFT methods: quantitative materials modeling at your fingertips	
11:45 – 13:45	<b>Photograph and Lunch</b>	<i>Ballroom/ Restaurant Maria Theresia (ground floor)</i>
<i>Session Chair: David Reith</i> 13:45 – 14:30	<b>Phuti Ngoepe</b> , University of Limpopo, South Africa Exploring minerals and energy storage with simulations	
14:30 – 15:15	<b>Ralf Drautz</b> , Ruhr-University of Bochum, Germany From high-throughput density functional theory to the simulation of materials with the atomic cluster expansion	
15:15 – 15:45 pm	<b>Coffee Break</b>	<i>Kaiserlounge (ground floor)</i>
<i>Session Chair: Mikael Christensen</i> 15:45 – 16:30	<b>Anders Engström</b> , Thermo-Calc Software, Solna, Sweden Bridging Atoms and Microstructure	
16:30 – 17:15	<b>Edwin Knobbe</b> , BMW, Munich, Germany, and <b>René Windiks</b> , Materials Design Bridging the canyon between atomistic and continuum modeling for battery cells	



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17:45 DEPART

**18:15 - 22:00** **Annual Customer Banquet** *Weitsicht Cobenzl (bus with MD guides)*

Wednesday, 11 October 2023

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6:00 - 9:00 am **Breakfast** *Restaurant Maria Theresia (ground floor)*

9:00 – 17:00 **Scientific Program** *Ballroom (ground floor)*

*Session Chair: Dave Rigby*  
9:00 – 9:45 **Thomas Pigeon**, IFP-EN, Lyon, France  
Computing catalytic reaction times and paths with machine learning and rare events sampling methods

9:45 – 10:15 **Jörg-Rüdiger Hill**, Materials Design  
Machine-learned potentials for eucryptite: A systematic comparison

10:15 – 10:30 **Coffee Break** *Kaiserlounge (ground floor)*

*Session Chair: Clive Freeman*  
10:30 – 11:00 **Marthe Bideault**, Materials Design, and **Ryoji Asahi**, Univ. of Nagoya, Japan  
Catalysis and the dynamics of nanoparticles

11:00 – 11:30 **Garrett Tow**, Materials Design  
Modeling and Understanding Solid Propellants

11:30 – 12:00 **Leonid Kahle and Kyle Starkey**, Materials Design,  
From the nanoscale to microstructures: a phase field approach

12:00 – 12:10 **Wrap-up and Conclusions**

12:15 – 14:00 **Lunch** *Restaurant Maria Theresia (ground floor)*

14:00 – 16:00 Informal discussions between MD and Customer

15:30 - 16:00 pm Coffee Break *Kaiserlounge (ground floor)*