



2023 Materials Design Users' Group Meeting

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

Saturday, 7 October 2023

No conference rooms or meals provided

Sunday, 8 October 2023

6:00 – 10:00	Breakfast	<i>Restaurant Maria Theresia (ground floor)</i>
11:00 - 11:30	Coffee Break	<i>Elisabeth Salon (downstairs)</i>
10:00 – 16:00	Set-Up (Training etc.)	<i>Franz Josef I (downstairs)</i>
12:30 – 13:30	Lunch Break	<i>Restaurant Maria Theresia (ground floor)</i>
<i>Schedule with Kathy</i>	Company portraits for anyone who is available	<i>(meet by front desk)</i>
<i>After set up optional coffee with team outside of the hotel.</i>		

No dinner provided

Monday, 9 October 2023

6:00 - 8:45	Breakfast	<i>Restaurant Maria Theresia (ground floor)</i>
8:30 - 17:00	Registration & Welcome Table	<i>Foyer near Ballroom (ground floor)</i>
9:00 - 17:00	UGM admin team	<i>Marie Room (4th floor)</i>
9:00 – 17:00	Meetings: Partners, Distributors, and MD	<i>Rudolf Room (5th 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>
17:00-18:00	Break-down Training Room	<i>Franz Josef I (downstairs)</i>
17:30	Poster Session Set-up	<i>Kaiserlounge (ground floor)</i>
18:30 - 21:00	Welcome Cocktail Reception and Poster Session	<i>Kaiserlounge (ground floor)</i>

Tuesday, 10 October 2023

6:00 - 9:00	Breakfast	<i>Restaurant Maria Theresia (ground floor)</i>
9:00 - 17:00	Registration & Welcome Table	<i>Ballroom (ground floor)</i>
9:00 - 17:00	UGM admin team	<i>Marie Room (4th floor)</i>
9:00 - 17:00	Meetings: Partners, Distributors, and MD	<i>Franz Josef I (downstairs)</i>
9:00 - 17:00	Meetings: Partners, Distributors, and MD	<i>Rudolf Room (5th 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	<i>Weitsicht Cobenzl (bus with MD guides)</i>



materials design®

Wednesday, 11 October 2023

6:00 - 9:00	Breakfast	<i>Restaurant Maria Theresia (ground floor)</i>
9:00 - 17:00	UGM admin team	<i>Marie Room (4th floor)</i>
9:00 – 17:00	Meetings: Partners, Distributors, and MD	<i>Rudolf Room (5th 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>
<i>TBD</i>	Individual Portraits (Please arrange with Kathy)	<i>(meet by front desk)</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>
18:20	Please assemble near front desk for journey to venue with MD guides	
18:30	Venue address: Motto am Fluss, Franz-Josefs-Kai 2 EG, 1010 Wien DEPART TOGETHER FOR THE 30 MIN TRAM– (RETURN ON YOUR OWN)	
19:00 –22:00	Company Dinner at the Restaurant Motto am Fluss	<i>Franz-Josefs-Kai 2 EG, 1010 Wien, Austria T +43 1 2525510 MD Guides for tram</i>

Thursday, 12 October 2023

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

TECHNICAL SESSIONS

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

6:00 - 9:00	Breakfast	<i>Restaurant Maria Theresia (ground floor)</i>
-------------	------------------	---

9:00 – 9:05	Erich Wimmer , Introduction and Session Chair
9:05 – 9:50	Michele Parrinello , Istituto Italiano di Tecnologia, Genoa, Italy The Solid State Physics of Catalysis
9:50 – 10:35	Saad Fahaid Khalaf Al-Afnan , 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	Coffee Break <i>Kaiserlounge (ground floor)</i>
<i>Session Chair: Volker Eyert</i> 11:00 – 11:45	Georg Kresse , University of Vienna, Austria Machine learning and Beyond DFT methods: quantitative materials modeling at your fingertips
11:45 – 13:45	Photograph and Lunch <i>Ballroom/ Restaurant Maria Theresia (ground floor)</i>
<i>Session Chair: David Reith</i> 13:45 – 14:30	Phuti Ngoepe , University of Limpopo, South Africa Exploring minerals and energy storage with simulations
14:30 – 15:15	Ralf Drautz , 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	Coffee Break <i>Kaiserlounge (ground floor)</i>
<i>Session Chair: Mikael Christensen</i> 15:45 – 16:30	Anders Engström , Thermo-Calc Software, Solna, Sweden Bridging Atoms and Microstructure
16:30 – 17:15	Edwin Knobbe , BMW, Munich, Germany, and René Windiks , Materials Design Bridging the canyon between atomistic and continuum modeling for battery cells
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

Wednesday, 11 October 2023

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, and **Wolfgang Mannstadt**, Schott AG, Mainz, Germany

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)

18:20

Please assemble near front desk for journey to venue with MD guides

Venue address: Motto am Fluss, Franz-Josefs-Kai 2 EG, 1010 Wien

18:30

DEPART

19:00 – 22:00

Company Dinner at the Restaurant Motto am Fluss

Franz-Josefs-Kai 2 EG,

1010 Wien, Austria

T +43 1 2525510

MD Guides for tram