

2019 Materials Design Users' Group Meeting

Austria Trend Parkhotel Schönbrunn
Vienna, Austria, 15 -17 October 2019

Monday, 14 October 2019

16:00	Hotel Check-in	<i>Reception Desk</i>
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No conference rooms or meals provided

Tuesday, 15 October 2019

6:00 - 9:00	Breakfast	<i>Restaurant Maria Theresia (ground floor)</i>
8:30 - 17:00	Registration & Welcome Table	<i>Ballroom (ground floor)</i>
9:00 - 17:00	Training Sessions	<i>Ballroom (ground floor)</i>
10:30 - 10:45	Coffee Break	<i>Bijou Bar (ground floor)</i>
12:30 - 13:30	Lunch Break	<i>Restaurant Maria Theresia (ground floor)</i>
15:30 - 15:45	Coffee Break	<i>Bijou Bar (ground floor)</i>
18:00	Poster Session Set-up	<i>Gloriette Bar (second floor)</i>
18:30 - 21:00	Welcome Cocktail Reception & Poster Session	<i>Gloriette Bar</i>

Wednesday, 16 October 2019

6:00 - 9:00	Breakfast	<i>Restaurant Maria Theresia (ground floor)</i>
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8:30 - 17:00	Registration & Welcome Table	<i>Ballroom (ground floor)</i>
9:00 - 17:20	Technical Sessions	<i>Ballroom (ground floor)</i>
10:30 - 10:50	Coffee Break	<i>Bijou Bar (ground floor)</i>
12:10 - 14:00	Official 2019 UGM Group Photo	Meet in Lobby
	Lunch	<i>Restaurant Maria Theresia (ground floor)</i>
15:30 - 16:00	Coffee Break	<i>Bijou Bar (ground floor)</i>
18:15	Please assemble in foyer for journey to venue with MD guides	Venue address: Hotel Sacher, Philharmonikerstraße 4, A-1010 Wien https://www.sacher.com/en/vienna/
19:00 - 22:00	Annual Customer Banquet	<i>Hotel Sacher MD Guides for subway</i>

Thursday, 17 October 2019

6:00 - 9:00	Breakfast	<i>Restaurant Maria Theresia (ground floor)</i>
9:00 - 12:30	Scientific Program	<i>Ballroom (ground floor)</i>
14:00 - 16:00	Informal discussions between MD and customers, partners and distributors	
10:20 - 10:40	Coffee Break	<i>Bijou Bar (ground floor)</i>



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12:30 - 14:00	Lunch	<i>Restaurant Maria Theresia (ground floor)</i>
16:00 - 16:30	Coffee Break	<i>Bijou Bar (ground floor)</i>
19:30 -22:00	Company Dinner at the Restaurant Griechenbeisl	<i>Fleischmarkt 11, 1010 Vienna T +43 1 533 1977 MD Guides for subway</i>

Friday, 18 October 2019

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

Scientific Program

Wednesday, 16 October 2019

All Technical Sessions - Ballroom (ground floor)

6:00 - 9:00

Breakfast

9:00 - 9:05

Erich Wimmer, Introduction and Session Chair

9:05 - 9:50

Georg Kresse, University of Vienna, Austria
Organic perovskites: from RPA to phase diagrams via machine learning

9:50 - 10:30

Moritz to Baben, GTT, Germany
Assessing phase stability with respect to competing phases

10:30 - 10:50

Coffee Break

Session Chair: Alexander Mavromaras

10:50 - 11:30

Antoine Claisse, Westinghouse, Sweden
Atomistic Modeling at Westinghouse - Needs and Perspectives

11:30 - 12:10

Richard W. Smith, Naval Nuclear Laboratory, USA
New Potentials for Zr/H: Collaboration with Materials Design, Inc.

12:10 - 14:00

Photograph and Lunch

Session Chair: Volker Eyert

14:00 - 14:20

Véronique Lachet, IFP-EN, France
Thermo-physical properties of $U_{1-y}Pu_yO_2$ MOX fuel using classical Monte Carlo simulations

14:20 - 15:00

Krzysztof Parlinski, University of Cracow, Poland
Phonon Anharmonicity from ab initio Calculations

15:00 - 15:30

Stéphane Brice Olou'ou Guifo, Volkswagen, Germany
Computational design of advanced energy materials for automotive engineering

15:30 - 16:00 pm

Coffee Break

Session Chair: Clive Freeman

16:00 - 16:40

Richard Catlow, Royal Society, UK
Computer Modelling of Nano-Particulate, Microporous, and Photo-active Catalysts



16:40 - 17:20

James J. P. Stewart, Stewart Computational Chemistry, USA

A worked example of how Computational Chemistry can help in solving an important and difficult problem

18:15

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<https://www.sacher.com/en/vienna/>

19:00 - 22:00

Customer Banquet at the Hotel Sacher

Thursday, 17 October 2019

6:00 - 9:00 am

Breakfast

9:00 - 17:00

Scientific Program

Session Chair: Dave Rigby

9:00 - 9:20

Ryan Thomas, Honeywell, USA

First-Principles Investigation of Hydrogen Trapping in Chemistry Dependent Vacancies of FeCrNi Alloys

9:20 - 9:40

Wes Everhart, Honeywell, USA

Applications of DFT to the ductility of intermetallic alloys

9:40 - 10:20

Marianna Yiannourakou, Materials Design, France

Predicting and Understanding Properties of Fluids with MedeA

10:20 - 10:40

Coffee Break

Session Chair: Erich Wimmer

10:40 - 11:20

Arthur France-Lanord, MIT, USA

Ion transport in polymer electrolytes: from theory to machine learning

11:20 - 12:30

Discussion and Conclusions

12:30 - 14:00

Lunch

14:00 - 16:00

Informal discussions between MD and customers, partners and distributors



Thank you for joining us at the Materials Design Users
Group Meeting this year!

Save the date for our next Users Group Meeting
in San Diego, California

Dates to be announced shortly

For more information and updates, follow us:

<https://www.materialsdesign.com/ugm-2019>