

# Agenda of DCTMD2024 (Drafted on June 22, 2024)

Dates: October 9-13, 2024

Venue: Grand Central Hotel Shanghai, Shanghai, China  
and Shanghai University (SHU), Shanghai, China

## Overview

- 6 Plenary talks, 30 mins each, including 5 min discussion
- 28 Invited talks, 20 mins each, including 3 min discussion
- 16 Contributed talks, 15 mins each, including 2 min discussion
- 50+ Posters (~20 poster awards),
- 1 Panel discussion 1, 40 mins including 4 questions
- 1 Tutorial, 5 hours

## Day 0: October 9, 2024 – Registration and Reception, Grand Central Hotel Shanghai

Time	Arrangement
1:00 PM - 8:00 PM	Arrival and registration at the hotel
5:00 PM - 8:00 PM	Buffet dinner at the hotel

## Day 1: October 10, 2024, Shanghai University (SHU)

### Morning Session (Plenary talk 1, invited talk 4)

Time	Arrangement
9:00 AM - 10:00 AM	Moving from the hotel to SHU (~1 hour by conference bus or subway)
10:00 AM - 10:25 AM	Opening Ceremony & Welcome Remarks
10:25 AM - 10:55 AM	<b>Plenary 1:</b> Speaker: Roberto Car (Princeton University, USA)
10:55 AM - 12:15 PM	Session 1-1: Machine-learned interatomic potential <b>I1-1:</b> Title <i>T. Daniel Crawford (Virginia Tech, USA)</i> <b>I1-2:</b> Title <i>Linfeng Zhang (DP Technology, China)</i> <b>I1-3:</b> “Accurate and efficient biomolecular dynamics enabled by machine-learned force fields” <i>Alexandre Tkatchenko (Luxembourg University, Luxembourg)</i> <b>I1-4:</b> “First-principles artificial intelligence” <i>Yong Xu (Tsinghua University, China)</i>

**Afternoon Session** (Plenary talk 1, invited talk 4, Panel discussion 1, Poster 50)

<b>Time</b>	<b>Arrangement</b>
12:15 PM - 1:30 PM:	Lunch Break; Video play at noon
1:30 PM - 2:00 PM	<b>Plenary 2:</b> Title <i>Yanming Ma (Jilin University, China)</i>
2:00 PM - 3:20 PM	Session 1-2: Automatic, autonomous, self-driving experiments <b>I1-5:</b> “Creating Synergies between Experimental and Computational Approaches in Advanced Materials Design: Importance and Challenges of Clean Data” <i>Annette Trunscke (FHI-Berlin, Germany)</i> <b>I1-6:</b> Title <i>Jun Jiang (USTC, China)</i> <b>I1-7:</b> Title <i>Keisuke Takahashi (Hokkaido University, Japan)</i> <b>I1-8:</b> Title <i>Jungho Shin (KRICT, South Korea)</i>
3:20 PM - 4:00 PM	<b>Panel Discussion:</b> "Unlocking the AI future of Materials Science" (40 min Panel discussions, four topics: Databases, Computations, AI algorithms, Autonomous experiments, 10 mins each) (Collection of oral discussions and written comments to form a future perspective on Data-driven materials design possibly published in a journal, e.g. Journal of Materials Informatics) Speakers: Xingao Gong (Fudan University), Hong Wang (Shanghai Jiaotong University), ...
4:00 PM - 5:00 PM	<b>Poster session</b> (~50+ posters)
5:00 PM - 6:30 PM	Moving from SHU to the Shanghai Bund (~1 hour by conference bus or subway)
6:30 - 9:00 PM	Dinner at the Shanghai Bund

**Day 2: October 11, 2024, Grand Central Hotel Shanghai****Morning Session** (Plenary talk 1, Invited talk 5, Contributed talk 4)

<b>Time</b>	<b>Arrangement</b>
8:45 AM - 9:15 AM	<b>Plenary 3:</b> Title <i>Berend Smit (EPFL, Switzerland)</i>
9:15 AM - 10:35 AM	Session 2-1: AI-guided materials design <b>I2-1:</b> “How Landau theory can guide data science to find materials with targeted response” <i>Turab Lookman (AiMaterials Research LLC, USA)</i> <b>I2-2:</b> “Polymer Informatics: Algorithmic Advances & Materials Design” <i>Rampi Ramprasad (Georgia Tech, USA)</i>

	<p><b>I2-3:</b> Title <i>Timon Rabczuk (The Bauhaus-Universität Weimar, Germany)</i></p> <p><b>I2-4:</b> “Machine learning based multiscale exploration and characterization of 2D materials” <i>Xiaoying Zhuang (Leibniz University Hannover, Germany)</i></p>
10:35 AM - 11:00 AM	Coffee Break
11:00 AM - 12:20 PM	<p>Session 2-2:</p> <p><b>I2-5:</b> “What do we mean by new? Quantifying structural uniqueness in the era of generative crystal structure prediction” <i>Taylor Sparks (The University of Utah, USA)</i></p> <p><b>C2-1:</b> “From computational screening to the synthesis of a promising OER catalyst” <i>Zhenpeng Yao (Shanghai Jiaotong University, China)</i></p> <p><b>C2-2:</b> Title <i>Speaker</i></p> <p><b>C2-3:</b> Title <i>Speaker</i></p> <p><b>C2-4:</b> Title <i>Speaker</i></p>

**Afternoon Session** (Plenary talk 1, Invited talk 5, Contributed talk 4)

<b>Time</b>	<b>Arrangement</b>
12:20 PM - 1:30 PM	Lunch Break
1:30 PM - 2:00 PM	<p>Plenary 4: Title Speaker: Chris Wolverton (Northwestern University, USA)</p>
2:00 PM - 3:20 PM	<p>Session 2-3: AI-assisted computational materials design</p> <p><b>I2-6:</b> Title <i>Zhipan Liu (Fudan University, China)</i></p> <p><b>I2-7:</b> “Accurate materials modeling by machine learning and beyond DFT methods” <i>Carla Verdi (The University of Queensland, Australia)</i></p> <p><b>I2-8:</b> “Advancing Molecular Simulations with Machine-Learned Interatomic Potentials” <i>Yangshuai Wang (National University of Singapore, Singapore)</i></p> <p><b>I2-9:</b> Title <i>Yuanyuan Zhou (DTU, Denmark)</i></p>
3:20 PM – 3:50 PM	Coffee Break
3:50 PM - 5:10 PM	<p>Session 2-4:</p> <p><b>I2-10:</b> Title <i>Lixue Cheng (Microsoft Research AI for Science Lab)</i></p> <p><b>C2-5:</b> Title</p>

	<i>Speaker</i> <b>C2-6:</b> Title <i>Speaker</i> <b>C2-7:</b> Title <i>Speaker</i> <b>C2-8:</b> Title <i>Speaker</i>
6:00-8:00 PM	Banquet at the Wangbaohe Hotel (5 min walk)

### Day 3: October 12, 2024, Grand Central Hotel Shanghai

#### Morning Session (Plenary talk 1, Invited talk 5, Contributed talk 4)

Time	Arrangement
8:45 AM - 9:15 AM	<b>Plenary 5:</b> “Describing Materials Properties and Functions via the “Materials Genes” Concept” Lucas Foppa (FHI-Berlin, Germany)
9:15 AM - 10:35 AM	Session 3-1: AI-assisted materials discovery <b>I3-1:</b> “Symbolic Regression in Materials Informatics: Applications and Challenges” <i>Runhai Ouyang (Shanghai University, China)</i> <b>I3-2:</b> Title <i>Sergey V. Levchenko (Skotech, Russia)</i> <b>I3-3:</b> “AI4Materials: From Simulation to Generation” <i>Hongxia Hao (Microsoft Research AI for Science)</i> <b>I3-4:</b> Title <i>Speaker</i>
10:35 AM - 11:00 AM	Coffee Break
11:00 AM - 12:20 PM	Session 3-2: <b>I3-5:</b> Title <i>Speaker</i> <b>C3-1:</b> Title <i>Speaker</i> <b>C3-2:</b> Title <i>Speaker</i> <b>C3-3:</b> Title <i>Speaker</i> <b>C3-4:</b> Title <i>Speaker</i>

#### Afternoon Session (Plenary talk 1, Invited talk 5, Contributed talk 4)

Time	Arrangement
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12:20 PM - 1:30 PM	Lunch Break
1:30 PM - 2:00 PM	<b>Plenary 6:</b> “AI Foundation models and Active Learning for Materials Discovery and Process Design” <i>Xiaonan Wang (Tsinghua University, China)</i>
2:00 PM - 3:20 PM	Session 3-3: Databases and large models <b>I3-6:</b> Title <i>Junfeng Qiao (EPFL, Switzerland)</i> <b>I3-7:</b> “Ontology and the role of semantics in the development of knowledge-based materials databases” <i>Lauren Takahashi (Hokkaido University, Japan)</i> <b>I3-8:</b> “Generating public datasets for chemistry” <i>Karmen Čondić-Jurkić (Open Molecular Software Foundation, New Zealand)</i> <b>I3-9:</b> Title <i>Speaker</i>
3:20 PM - 3:50 PM	Coffee Break
3:50 PM - 5:10 PM	Session 3-4: <b>I3-10:</b> Title <i>Speaker</i> <b>C3-5:</b> Title <i>Speaker</i> <b>C3-6:</b> Title <i>Speaker</i> <b>C3-7:</b> Title <i>Speaker</i> <b>C3-8:</b> Title <i>Speaker</i>
5:10 PM - 5:40 PM	Closing Ceremony: Awards, Summary & Farewell Remarks
6:00 PM - 8:00 PM	Buffet dinner at the hotel

#### Day 4: October 13, 2024 Tutorial (optional) at Shanghai University (SHU) and Departure

Time	Arrangement
8:30 AM - 9:30 AM	Moving from the hotel to SHU (~1 hour by conference bus or subway)
9:30 AM - 5:00 PM	<b>Tutorial:</b> DeepMD: from algorithms to applications <i>Yibo Wang (DP Technology, China) et al.</i>

Website of the DeepMD tutorial (Introduction and Registration):

<https://bohrium.dp.tech/courses/1347727500?tab=courses&lang=en-us>

Time	Topic
09:30 - 10:30	Machine Learning Potentials: From DeePMD to DPA-2
10:30 - 11:30	Introduction to DeePMD-kit & DP-GEN
11:30 - 12:00	DeePMD-kit hands-on
13:00 - 14:30	Applications of DeePMD in Materials Research
14:30 - 16:00	Open Large Atomic Model: Advances in Alloy Research
16:00 - 17:00	Q&A Session

Note: The DeepMD tutorial has limited seats and needs additional registration. The tutorial is free for the registered participants at DCTMD (course materials and instruction in English).

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Note: This agenda is subject to adjustments. For updates, speaker details, and session topics, please visit [International workshop on data-driven computational and theoretical materials design \(scievent.com\)](https://dctmd2024.scievent.com/) (<https://dctmd2024.scievent.com/>).