Agenda of DCTMD2024 (Draft by June 22, 2024)

Overview: Plenary talks 6 (30 mins each, including 5 min discussion), invited talks 28 (20 mins each, including 3 min discussion), contributed talks 16 (15 mins each, including 2 min d iscussion), poster 50+ (~20 poster awards), panel discussion 1 (40 mins including 4 questions), and tutorial 1 (5 hours)

Dates: October 9-13, 2024
Venue: Grand Central Hotel Shanghai, Shanghai, China
and Shanghai University (SHU), Shanghai, China

Day 0: October 9, 2024 – Registration and Reception, Grand Central Hotel Shanghai
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)
● 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: Plenary 1:
Speaker: Roberto Car (Princeton University, USA)
(1 plenary talk, 30 min including 5 min discussions)
● 10:55 AM - 12:15 PM: Session 1-1: Machine-learned interatomic potential
(4 invited talks, 20 min each including 3 min discussions)
I1-1: TBD
Speaker: T. Daniel Crawford (Virginia Tech, USA)
I1-2: TBD
Speaker: Linfeng Zhang (DP Technology, China)
I1-3: "Accurate and efficient biomolecular dynamics enabled by machine-learned force fields"
Speaker: Alexandre Tkatchenko (Luxembourg University, Luxembourg)
I1-4: "First-principles artificial intelligence"
Speaker：Yong Xu (Tsinghua University, China)

➢ **Afternoon Session** (Plenary talk 1, invited talk 4, Panel discussion 1, Poster 50)
● 12:15 PM - 1:30 PM: Lunch Break; Video play at noon
● 1:30 PM - 2:00 PM: Plenary 2: TBD
Speaker: Yanming Ma (Jilin University, China)
● 2:00 PM - 3:20 PM: Session 1-2: Automatic, autonomous, self-driving experiments

(4 invited talks, 20 min each including 3 min discussions)

I1-5: "Creating Synergies between Experimental and Computational Approaches in Advanced Materials Design: Importance and Challenges of Clean Data"

Speaker: Annette Trunscke (Fritz Haber Institute (FHI) of the Max Planck Society, Germany)

I1-6: TBD

Speaker: Jun Jiang (University of Science and Technology of China, China)

I1-7: TBD

Speaker: Keisuke Takahashi (Hokkaidao University, Japan)

I1-8: TBD

Speaker：Jungho Shin (Korea Research Institute of Chemical Technology, South Korea)

- 3:20 PM - 4:00 PM: Panel Discussion: "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)

- 4:00 PM - 5:00 PM: Poster session (~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)

- 8:45 AM - 9:15 AM: Plenary 3: TBD

Speaker: Berend Smit (Swiss Federal Institute of Technology in Lausanne (EPFL), Switzerland)

- 9:15 AM - 10:35 AM: Session 2-1: AI-guided materials design

(4 invited talks, 20 min each including 3 min discussions)

I2-1: "How Landau theory can guide data science to find materials with targeted response"

Speaker: Turab Lookman (AiMaterials Research LLC, USA)

I2-2: "Polymer Informatics: Algorithmic Advances & Materials Design"

Speaker: Rampi Ramprasad (Georgia Tech, USA)

I2-3: TBD

Speaker: Timon Rabczuk (The Bauhaus-Universität Weimar, Germany)

I2-4: "Machine learning based multiscale exploration and characterization of 2D materials"

Speaker: Xiaoying Zhuang (Leibniz University Hannover, Germany)

- 10:35 AM - 11:00 AM: Coffee Break

- 11:00 AM - 12:20 PM: Session 2-2:

(1 invited talks, 20 min each including 3 min discussions)

(4 contributed talks, 15 min each including 2 min discussions)

I2-5: "What do we mean by new? Quantifying structural uniqueness in the era of generative crystal structure prediction"

Speaker: Taylor Sparks (The University of Utah, USA)

C2-1: "From computational screening to the synthesis of a promising OER catalyst"

Speaker: Zhenpeng Yao (Shanghai Jiaotong University, China)

C2-2: TBD

Speaker: TBD

C2-3: TBD

Speaker: TBD

C2-4: TBD

Speaker: TBD

➢ **Afternoon Session** (Plenary talk 1, Invited talk 5, Contributed talk 4)
- 12:20 PM - 1:30 PM: Lunch Break
- 1:30 PM - 2:00 PM: Plenary 4: TBD

Speaker: Chris Wolverton (Northwestern University, USA)
- 2:00 PM - 3:20 PM: Session 2-3: AI-assisted computational materials design

(4 invited talks, 20 min each including 3 min discussions)

I2-6: TBD

Speaker: Zhipan Liu (Fudan University, China)

I2-7: "Accurate materials modeling by machine learning and beyond DFT methods"

Speaker: Carla Verdi (The University of Queensland, Australia)

I2-8: "Advancing Molecular Simulations with Machine-Learned Interatomic Potentials"

Speaker: Yangshuai Wang (Department of Mathematics, National University of Singapore, Singapore)

I2-9: TBD

Speaker: Yuanyuan Zhou (Technical University of Denmark (DTU), Denmark)
- 3:20 PM – 3:50 PM: Coffee Break
- 3:50 PM - 5:10 PM: Session 2-4:

(1 invited talks, 20 min each including 3 min discussions)

(4 contributed talks, 15 min each including 2 min discussions)

I2-10: TBD

Speaker: Lixue Cheng (Microsoft Research AI for Science Lab)

C2-5: TBD

Speaker: TBD

C2-6: TBD

Speaker: TBD

C2-7: TBD

Speaker: TBD

C2-8: TBD

Speaker: TBD

- 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)

- 8:45 AM - 9:15 AM: Plenary 5: "Describing Materials Properties and Functions via the "Materials Genes" Concept"

Speaker: Lucas Foppa (Fritz Haber Institute (FHI) of the Max Planck Society, Germany)

- 9:15 AM - 10:35 AM: Session 3-1: AI-assisted materials discovery

(4 invited talks, 20 min each including 3 min discussions)

I3-1: "Symbolic Regression in Materials Informatics: Applications and Challenges"

Speaker: Runhai Ouyang (Shanghai University, China)

I3-2: TBD

Speaker: Sergey V. Levchenko (Skolkovo Institute of Science and Technology (Skotech), Russia)

I3-3: "AI4Materials: From Simulation to Generation"

Speaker: Hongxia Hao (Microsoft Research AI for Science)

I3-4: TBD

Speaker: TBD

- 10:35 AM - 11:00 AM: Coffee Break
- 11:00 AM - 12:20 PM: Session 3-2:

(1 invited talks, 20 min each including 3 min discussions)

(4 contributed talks, 15 min each including 2 min discussions)

I3-5: TBD

Speaker: TBD

C3-1: TBD

Speaker: TBD

C3-2: TBD

Speaker: TBD

C3-3: TBD

Speaker: TBD

C3-4: TBD

Speaker: TBD

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

- 12:20 PM - 1:30 PM: Lunch Break
- 1:30 PM - 2:00 PM: Plenary 6: "AI Foundation models and Active Learning for Materials Discovery and Process Design"

Speaker: Xiaonan Wang (Tsinghua University, China)

- 2:00 PM - 3:20 PM: Session 3-3: Databases and large models

(4 invited talks, 20 min each including 3 min discussions)

I3-6: TBD

Speaker: Junfeng Qiao (Swiss Federal Institute of Technology in Lausanne (EPFL), Switzerland)

I3-7: "Ontology and the role of semantics in the development of knowledge-based materials databases"

Speaker: Lauren Takahashi (Hokkaido University, Japan)

I3-8: "Generating public datasets for chemistry"

Speaker: Karmen Čondić-Jurkić (Open Molecular Software Foundation, New Zealand)

I3-9: TBD

Speaker: TBD

3:20 PM - 3:50 PM: Coffee Break

3:50 PM - 5:10 PM: Session 3-4:

(1 invited talks, 20 min each including 3 min discussions)

(4 contributed talks, 15 min each including 2 min discussions)

I3-10: TBD

Speaker: TBD

C3-5: TBD

Speaker: TBD

C3-6: TBD

Speaker: TBD

C3-7: TBD

Speaker: TBD

C3-8: TBD

Speaker: TBD

- 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 at Shanghai University (SHU) and Departure
- 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: Tutorial: DeepMD: from algorithms to applications

Speaker: Yibo Wang (DP Technology, China) and other instructors

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).

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/).