

# Agenda of the International Workshop on Data-Driven Computational and Theoretical Materials Design (DCTMD2024)

(Dated on Sep. 11, 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> Title <i>Roberto Car (Princeton University, USA)</i>
10:55 AM - 12:15 PM	Session 1-1: Machine-learned interatomic potential <b>I1-1:</b> “The Molecular Sciences Software Institute” <i>T. Daniel Crawford (Virginia Tech, USA)</i> <b>I1-2:</b> Title <i>Linfeng Zhang (DP Technology, China)</i> <b>I1-3:</b> “Recent advances in Deep QMC developments and its molecular property calculations” <i>Lixue Cheng (Microsoft Research AI for Science Lab)</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, 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 submitted a journal, e.g. Journal of Materials Informatics) Speakers: <i>Hong Wang (Shanghai Jiaotong University), ...</i>
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> “Data Science to Optimize Metal-Organic Frameworks for Carbon Capture Applications” <i>Berend Smit (EPFL, Switzerland)</i>
9:15 AM - 10:35 AM	Session 2-1: AI-guided materials design <b>I2-1:</b> “Guiding the next experiment: Bayesian Global Optimization versus Reinforcement Learning” <i>Turab Lookman (AiMaterials Research LLC, USA)</i> <b>I2-2:</b> “Polymer Informatics: Algorithmic Advances & Materials Design”

	<p><i>Rampi Ramprasad (Georgia Tech, USA)</i>  <b>I2-3:</b> Title  <i>Timon Rabczuk (The Bauhaus-Universität Weimar, Germany)</i>  <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:  <b>I2-5:</b> “AI4Materials: From Simulation to Generation”  <i>Hongxia Hao (Microsoft Research AI for Science)</i>  <b>C2-1:</b> “From computational screening to the synthesis of a promising OER catalyst”  <i>Zhenpeng Yao (Shanghai Jiaotong University, China)</i>  <b>C2-2:</b> “From imaginary phonons to a universal interatomic potential: the case of BiFeO<sub>3</sub>”  <i>Bastien F. Grosso (University of Birmingham, United Kingdom)</i>  <b>C2-3:</b> “Computational modeling and simulation of molecular design and property prediction of novel elastomer materials”  <i>Jun Liu (Beijing University of Chemical Technology, Beijing, China)</i>  <b>C2-4:</b> “Progress in Machine Learning Studies for High-Entropy Alloys”  <i>Guangcun Shan (Beihang University, Beijing, China)</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  <i>Chris Wolverton (Northwestern University, USA)</i></p>
2:00 PM - 3:20 PM	<p>Session 2-3: AI-assisted computational materials design  <b>I2-6:</b> Title  <i>Zhipan Liu (Fudan University, China)</i>  <b>I2-7:</b> “Accurate materials modeling by machine learning and beyond DFT methods”  <i>Carla Verdi (The University of Queensland, Australia)</i>  <b>I2-8:</b> “Advancing Molecular Simulations with Machine-Learned Interatomic Potentials”  <i>Yangshuai Wang (National University of Singapore, Singapore)</i>  <b>I2-9:</b> “Accurate and efficient biomolecular dynamics enabled by machine-learned force fields”  <i>Alexandre Tkatchenko (Luxembourg University, Luxembourg)</i></p>
3:20 PM – 3:50 PM	Coffee Break
3:50 PM - 5:10 PM	Session 2-4:

	<p><b>I2-10:</b> “Data-Enabled Synthesis Predictions for Molecules and Materials” <i>Yousung Jung (Seoul National University, Korea)</i></p> <p><b>C2-5:</b> “HH130: A Standardized Dataset for Universal Machine Learning Force Field and the Applications in the Thermal Transport of Half-Heusler Thermoelectrics” <i>Jiong Yang (Shanghai University, Shanghai, China)</i></p> <p><b>C2-6:</b> “Bayesian Optimization for High-Resolution Transmission Electron Microscopy” <i>Xiankang Tang (TU Darmstadt, Germany)</i></p> <p><b>C2-7:</b> “Anisotropic materials with abnormal Poisson's ratios and acoustic velocities” <i>Chunxia Chi (Nankai University, China)</i></p> <p><b>C2-8:</b> “Effective lattice potentials of perovskite oxides derived from elaborately designed training dataset” <i>Huazhang Zhang (University of Liège, Belgium)</i></p>
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	<p><b>Plenary 5:</b> “Describing Materials Properties and Functions via the “Materials Genes” Concept” <i>Lucas Foppa (Fritz Haber Institute of the Max-Planck-Gesellschaft, Germany)</i></p>
9:15 AM - 10:35 AM	<p>Session 3-1: AI-assisted materials discovery</p> <p><b>I3-1:</b> “Symbolic Regression in Materials Informatics: Applications and Challenges” <i>Runhai Ouyang (Shanghai University, Shanghai, China)</i></p> <p><b>I3-2:</b> “Finding Descriptors of Catalytic Properties from Data for Catalyst Design with the Help of Artificial Intelligence” <i>Sergey V. Levchenko (Skotech, Russia)</i></p> <p><b>I3-3:</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>I3-4:</b> “AI-accelerated grand-canonical method for surface processes” <i>Yuanyuan Zhou (DTU, Denmark)</i></p>
10:35 AM - 11:00 AM	Coffee Break
11:00 AM - 12:20 PM	<p>Session 3-2:</p> <p><b>I3-5:</b> “Language Data-Driven Machine Learning Design of New</p>

	<p>Materials”</p> <p><i>Lei Zhang (Nanjing University of Information Science and Technology, Nanjing, China)</i></p> <p><b>C3-1:</b> “Extraction of data from publications empowered by Kolmogorov-Arnold Networks”</p> <p><i>Wenkai Ning (Shanghai University, Shanghai, China)</i></p> <p><b>C3-2:</b> “AI-driven Workflow for Identifying Stable Oxides for Electrocatalysis”</p> <p><i>Akhil S. Nair (Fritz Haber Institute of the Max-Planck-Gesellschaft, Germany)</i></p> <p><b>C3-3:</b> “Adapting Explainable Machine Learning to Study Mechanical Properties of Two-Dimensional Hybrid Halide Perovskites”</p> <p><i>Dan Han (Jilin University, Changcun, China)</i></p> <p><b>C3-4:</b> “Battery prognosis from impedance spectroscopy using machine learning”</p> <p><i>Yunwei Zhang (Sun Yat-sen University, Guangzhou, China)</i></p>
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#### Afternoon Session (Plenary talk 1, Invited talk 5, Contributed talk 4)

Time	Arrangement
12:20 PM - 1:30 PM	Lunch Break
1:30 PM - 2:00 PM	<p><b>Plenary 6:</b> “AI Foundation models and Active Learning for Materials Discovery and Process Design”</p> <p><i>Xiaonan Wang (Tsinghua University, China)</i></p>
2:00 PM - 3:20 PM	<p>Session 3-3: Databases and large models</p> <p><b>I3-6:</b> “The Electronic-Structure Genome of Inorganic Crystals”</p> <p><i>Junfeng Qiao (EPFL, Switzerland)</i></p> <p><b>I3-7:</b> “Ontology and the role of semantics in the development of knowledge-based materials databases”</p> <p><i>Lauren Takahashi (Hokkaido University, Japan)</i></p> <p><b>I3-8:</b> “A Large Multi-Modality Model for Chemistry and Materials Science”</p> <p><i>Xin Chen (Suzhou Laboratory, Suzhou, China)</i></p> <p><b>I3-9:</b> “Unexpected Failure and Success in Data-Driven Materials Science”</p> <p><i>Kangming Li (University of Toronto, Canada)</i></p>
3:20 PM - 3:50 PM	Coffee Break
3:50 PM - 5:10 PM	<p>Session 3-4:</p> <p><b>I3-10:</b> “Scalable Crystal Structure Relaxation Using an Iteration-free Deep Generative Model with Uncertainty Quantification”</p> <p><i>Lei Shen (National University of Singapore, Singapore)</i></p>

	<p><b>C3-5:</b> “Simulating the Microscopic World: From Schrödinger Equation to Large Atomic Models”  <i>Han Wang (Institute of Applied Physics and Computational Mathematics, Beijing, China)</i></p> <p><b>C3-6:</b> “Leveraging Open-Access Libraries for Feature Engineering in Material Discovery”  <i>Mohammad Khatamirad (BasCat–UniCat BASF JointLab, Technical University of Berlin, Berlin, Germany)</i></p> <p><b>C3-7:</b> Title  <i>Speaker</i></p> <p><b>C3-8:</b> Title  <i>Speaker</i></p>
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 et al. (DP Technology, China)</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).

Note: This agenda including the presentation types is subject to adjustments after evaluation by the organization committee. For updates, speaker details, and session topics, please visit [International workshop on data-driven computational and theoretical materials design \(scievent.com\)](https://www.scievent.com)

(<https://dctmd2024.scievent.com/>).