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

(Dated on Sep. 10, 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	**Plenary 1**: Title *Roberto Car (Princeton University, USA)*
10:55 AM - 12:15 PM	Session 1-1: Machine-learned interatomic potential **I1-1**: "The Molecular Sciences Software Institute" *T. Daniel Crawford (Virginia Tech, USA)* **I1-2**: Title *Linfeng Zhang (DP Technology, China)* **I1-3**: "Recent advances in Deep QMC developments and its molecular property calculations" *Lixue Cheng (Microsoft Research AI for Science Lab)* **I1-4**: "First-principles artificial intelligence" *Yong Xu (Tsinghua University, China)*

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

Time	Arrangement
12:15 PM - 1:30 PM:	Lunch Break; Video play at noon
1:30 PM - 2:00 PM	**Plenary 2**: Title *Yanming Ma (Jilin University, China)*
2:00 PM - 3:20 PM	Session 1-2: Automatic, autonomous, self-driving experiments **I1-5**: "Creating Synergies between Experimental and Computational Approaches in Advanced Materials Design: Importance and Challenges of Clean Data" *Annette Trunscke (FHI-Berlin, Germany)* **I1-6**: Title *Jun Jiang (USTC, China)* **I1-7**: Title *Keisuke Takahashi (Hokkaidao University, Japan)* **I1-8**: Title *Jungho Shin (KRICT, 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 submitted a journal, e.g. Journal of Materials Informatics) Speakers: *Hong Wang (Shanghai Jiaotong University)*, …
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)

Time	Arrangement
8:45 AM - 9:15 AM	**Plenary 3**: "Data Science to Optimize Metal-Organic Frameworks for Carbon Capture Applications" *Berend Smit (EPFL, Switzerland)*
9:15 AM - 10:35 AM	Session 2-1: AI-guided materials design **I2-1**: "Guiding the next experiment: Bayesian Global Optimization versus Reinforcement Learning" *Turab Lookman (AiMaterials Research LLC, USA)* **I2-2**: "Polymer Informatics: Algorithmic Advances & Materials Design"

	Rampi Ramprasad (Georgia Tech, USA) **I2-3**: Title *Timon Rabczuk (The Bauhaus-Universität Weimar, Germany)* **I2-4**: "Machine learning based multiscale exploration and characterization of 2D materials" *Xiaoying Zhuang (Leibniz University Hannover, Germany)*
10:35 AM - 11:00 AM	Coffee Break
11:00 AM - 12:20 PM	Session 2-2: **I2-5**: "What do we mean by new? Quantifying structural uniqueness in the era of generative crystal structure prediction" *Taylor Sparks (The University of Utah, USA)* **C2-1**: "From computational screening to the synthesis of a promising OER catalyst" *Zhenpeng Yao (Shanghai Jiaotong University, China)* **C2-2**: "From imaginary phonons to a universal interatomic potential: the case of $BiFeO_3$" *Bastien F. Grosso (University of Birmingham, United Kingdom)* **C2-3**: "Computational modeling and simulation of molecular design and property prediction of novel elastomer materials" *Jun Liu (Beijing University of Chemical Technology, Beijing, China)* **C2-4**: "Progress in Machine Learning Studies for High-Entropy Alloys" *Guangcun Shan (Beihang University, Beijing, China)*

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	Plenary 4: Title *Chris Wolverton (Northwestern University, USA)*
2:00 PM - 3:20 PM	Session 2-3: AI-assisted computational materials design **I2-6**: Title *Zhipan Liu (Fudan University, China)* **I2-7**: "Accurate materials modeling by machine learning and beyond DFT methods" *Carla Verdi (The University of Queensland, Australia)* **I2-8**: "Advancing Molecular Simulations with Machine-Learned Interatomic Potentials" *Yangshuai Wang (National University of Singapore, Singapore)* **I2-9**: "Accurate and efficient biomolecular dynamics enabled by machine-learned force fields" *Alexandre Tkatchenko (Luxembourg University, Luxembourg)*
3:20 PM – 3:50 PM	Coffee Break

3:50 PM - 5:10 PM	Session 2-4: **I2-10**: "Data-Enabled Synthesis Predictions for Molecules and Materials" *Yousung Jung (Seoul National University, Korea)* **C2-5**: "HH130: A Standardized Dataset for Universal Machine Learning Force Field and the Applications in the Thermal Transport of Half-Heusler Thermoelectrics" *Jiong Yang (Shanghai University, Shanghai, China)* **C2-6**: "Bayesian Optimization for High-Resolution Transmission Electron Microscopy" *Xiankang Tang (TU Darmstadt, Germany)* **C2-7**: "Anisotropic materials with abnormal Poisson's ratios and acoustic velocities" *Chunxia Chi (Nankai University, China)* **C2-8**: "Effective lattice potentials of perovskite oxides derived from elaborately designed training dataset" *Huazhang Zhang (University of Liège, Belgium)*
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	**Plenary 5**: "Describing Materials Properties and Functions via the "Materials Genes" Concept" *Lucas Foppa (Fritz Haber Institute of the Max-Planck-Gesellschaft, Germany)*
9:15 AM - 10:35 AM	Session 3-1: AI-assisted materials discovery **I3-1**: "Symbolic Regression in Materials Informatics: Applications and Challenges" *Runhai Ouyang (Shanghai University, Shanghai, China)* **I3-2**: "Finding Descriptors of Catalytic Properties from Data for Catalyst Design with the Help of Artificial Intelligence" *Sergey V. Levchenko (Skotech, Russia)* **I3-3**: "AI4Materials: From Simulation to Generation" *Hongxia Hao (Microsoft Research AI for Science)* **I3-4**: "AI-accelerated grand-canonical method for surface processes" *Yuanyuan Zhou (DTU, Denmark)*
10:35 AM - 11:00 AM	Coffee Break
11:00 AM - 12:20 PM	Session 3-2: **I3-5**: "Language Data-Driven Machine Learning Design of New

	Materials” *Lei Zhang (Nanjing University of Information Science and Technology, Nanjing, China)* **C3-1**: “Extraction of data from publications empowered by Kolmogorov-Arnold Networks” *Wenkai Ning (Shanghai University, Shanghai, China)* **C3-2**: “AI-driven Workflow for Identifying Stable Oxides for Electrocatalysis” *Akhil S. Nair (Fritz Haber Institute of the Max-Planck-Gesellschaft, Germany)* **C3-3**: “Battery prognosis from impedance spectroscopy using machine learning” *Yunwei Zhang (Sun Yat-sen University, Guangzhou, China)* **C3-4**: Title *Speaker*

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	**Plenary 6**: “AI Foundation models and Active Learning for Materials Discovery and Process Design” *Xiaonan Wang (Tsinghua University, China)*
2:00 PM - 3:20 PM	Session 3-3: Databases and large models **I3-6**: “The Electronic-Structure Genome of Inorganic Crystals” *Junfeng Qiao (EPFL, Switzerland)* **I3-7**: “Ontology and the role of semantics in the development of knowledge-based materials databases” *Lauren Takahashi (Hokkaido University, Japan)* **I3-8**: “A Large Multi-Modality Model for Chemistry and Materials Science” *Xin Chen (Suzhou Laboratory, Suzhou, China)* **I3-9**: “Unexpected Failure and Success in Data-Driven Materials Science” *Kangming Li (University of Toronto, Canada)*
3:20 PM - 3:50 PM	Coffee Break
3:50 PM - 5:10 PM	Session 3-4: **I3-10**: “Scalable Crystal Structure Relaxation Using an Iteration-free Deep Generative Model with Uncertainty Quantification” *Lei Shen (National University of Singapore, Singapore)* **C3-5**: “Simulating the Microscopic World: From Schrödinger Equation

	to Large Atomic Models" *Han Wang (Institute of Applied Physics and Computational Mathematics, Beijing, China)* **C3-6**: Title *Speaker* **C3-7**: Title *Speaker* **C3-8**: Title *Speaker*
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	**Tutorial**: "DeepMD: from algorithms to applications" *Yibo Wang et al. (DP Technology, China)*

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://dctmd2024.scievent.com/).