

CyberMAGICS Workshop

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June 30, 2022



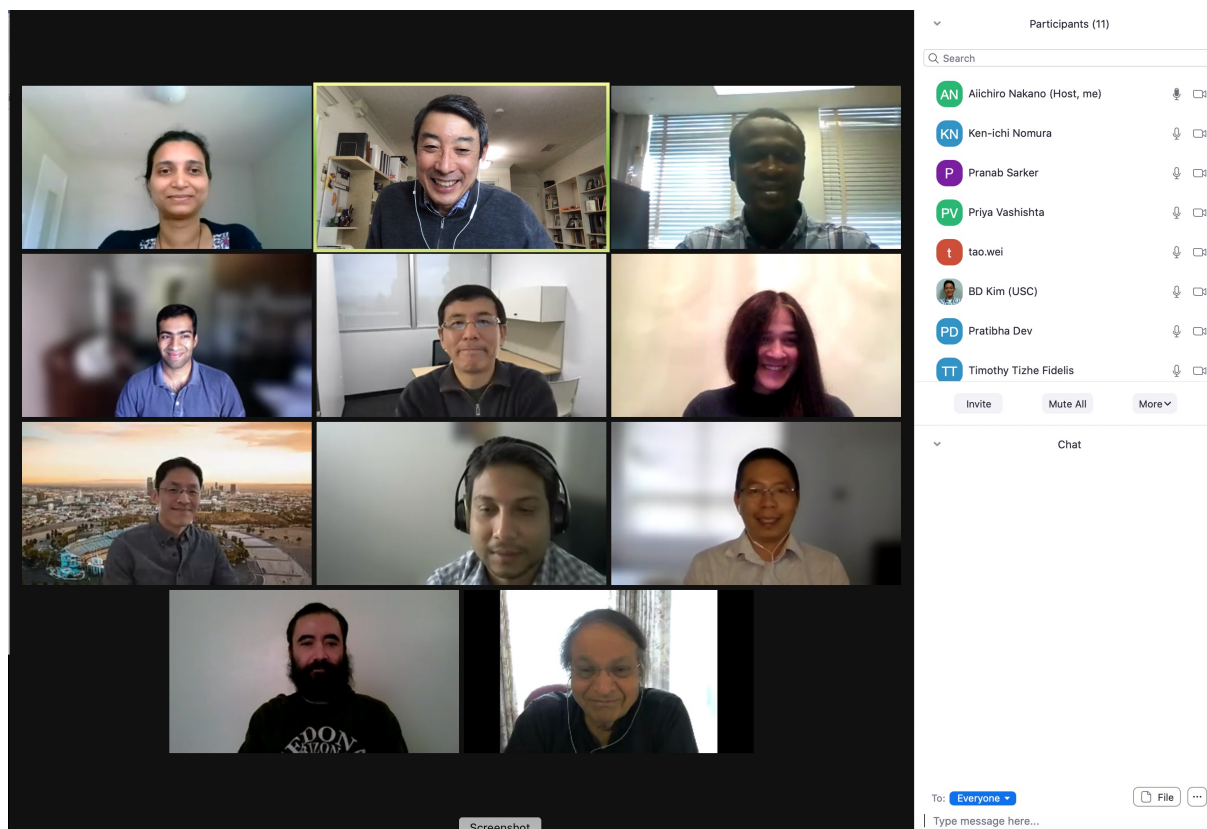
**HOWARD
UNIVERSITY**



USC-Howard Cybertraining

CyberMAGICS: Cyber Training on Materials Genome Innovation for Computational Software

- This project trains a new generation of materials cyberworkforce, who will solve challenging materials genome* problems through innovative use of advanced cyberinfrastructure at the exa-quantum-AI nexus



***Materials genome:**
Applying informatics to design new materials significantly faster than the conventional trial-and-error approach

NSF CyberTraining (2021-25) project

Nakano, Nomura, Vashishta (USC); Dev, Wei (Howard)

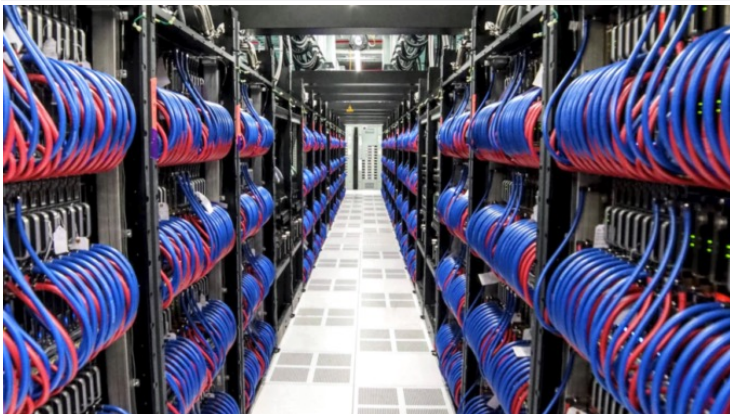
Exaflop/s Computer Has Just Arrived!

ORNL's Frontier First to Break the Exaflop Ceiling

May 30, 2022

The 59th edition of the TOP500 revealed the Frontier system to be the first true exascale machine with an HPL score of 1.102 Exaflop/s.

The No. 1 spot is now held by the Frontier system at Oak Ridge National Laboratory (ORNL) in the US. Based on the latest HPE Cray EX235a architecture and equipped with AMD EPYC 64C 2GHz processors, the system has 8,730,112 total cores, a power efficiency rating of 52.23 gigaflops/watt, and relies on gigabit ethernet for data transfer.



Exaflop/s: 10^{18} floating-point operations per second

<https://www.top500.org>

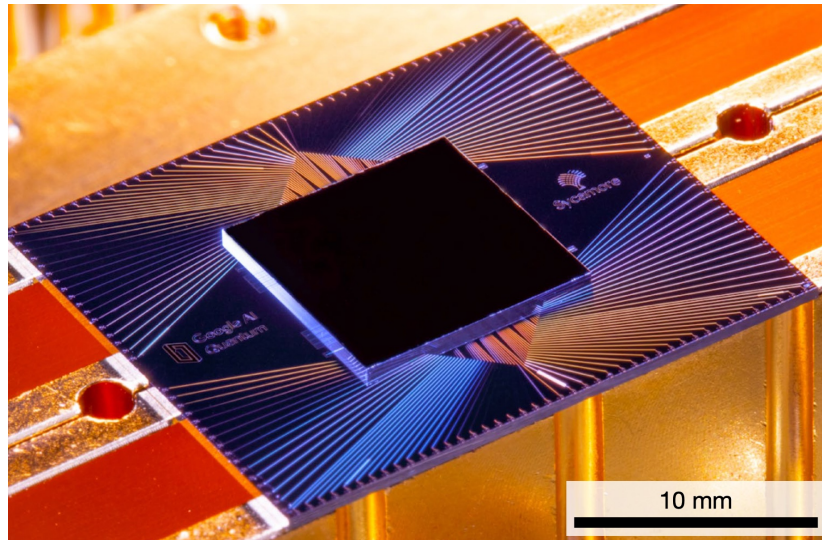
Changing Computing Landscape for Science

Postexascale Computing for Science



Compute Cambrian explosion

Quantum Computing for Science



AI for Science

DOE readies multibillion- dollar AI push

U.S. supercomputing leader
is the latest big backer
in a globally crowded field

By **Robert F. Service**, in Washington, D.C.

Science **366**, 559 (Nov. 1, '19)

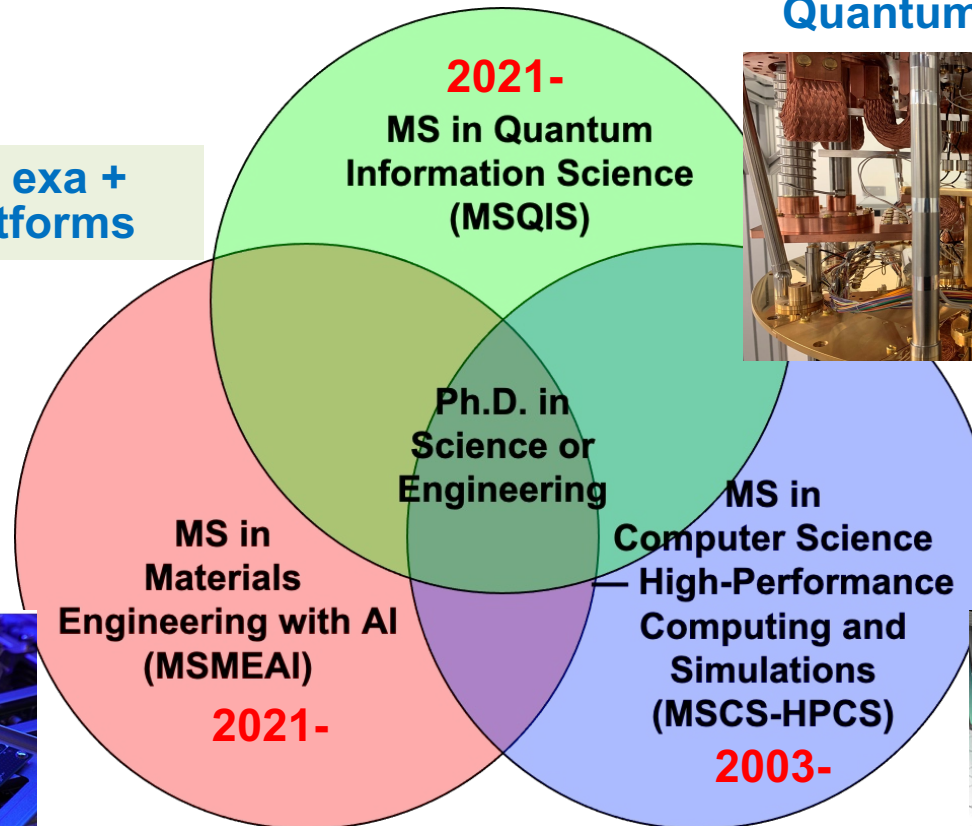


Use all to advance science!

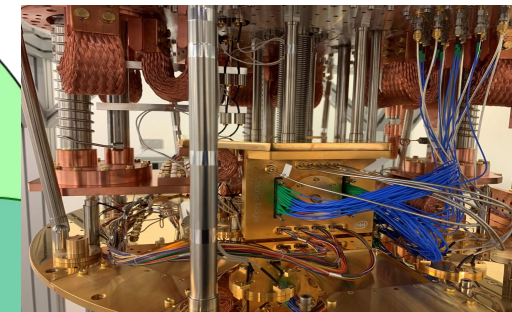
Training Cyber Science Workforce

- New generation of computational scientists at the **nexus of exascale computing, quantum computing & AI**
- **Unique dual-degree program at USC:** Ph.D. in materials science or physics, along with MS in computer science specialized in high-performance computing & simulations, MS in quantum information science or MS in materials engineering with AI

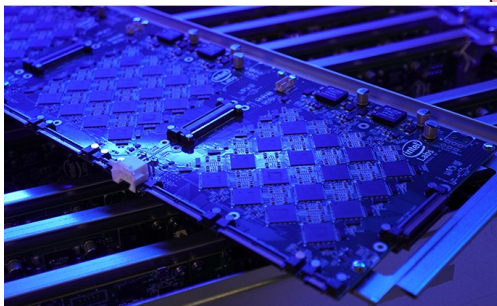
Cybertraining on exa + quantum + AI platforms



Horse Ridge II
Quantum computer



Neuromorphic
Pohoiki Springs

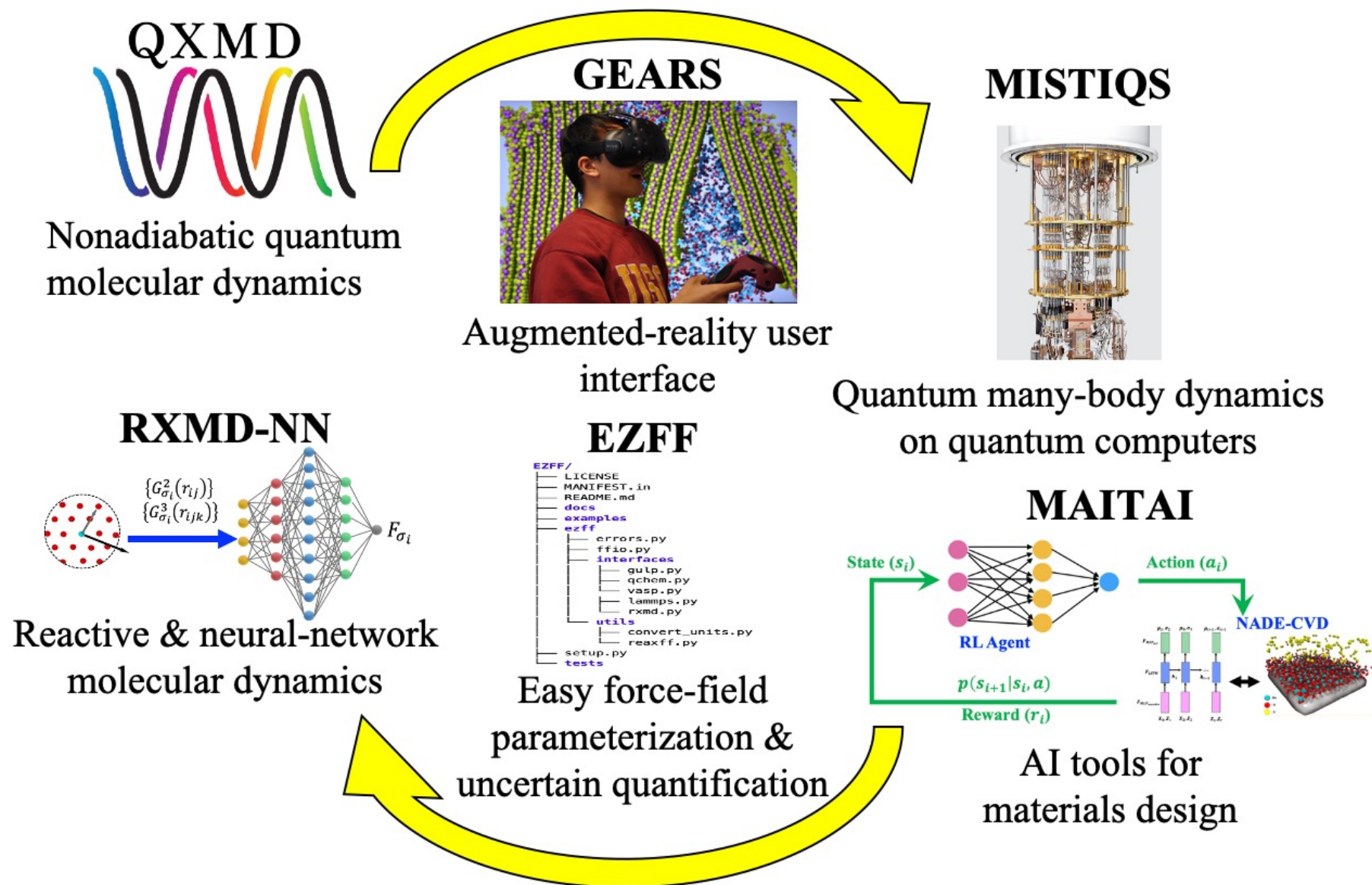


Exascale
Aurora



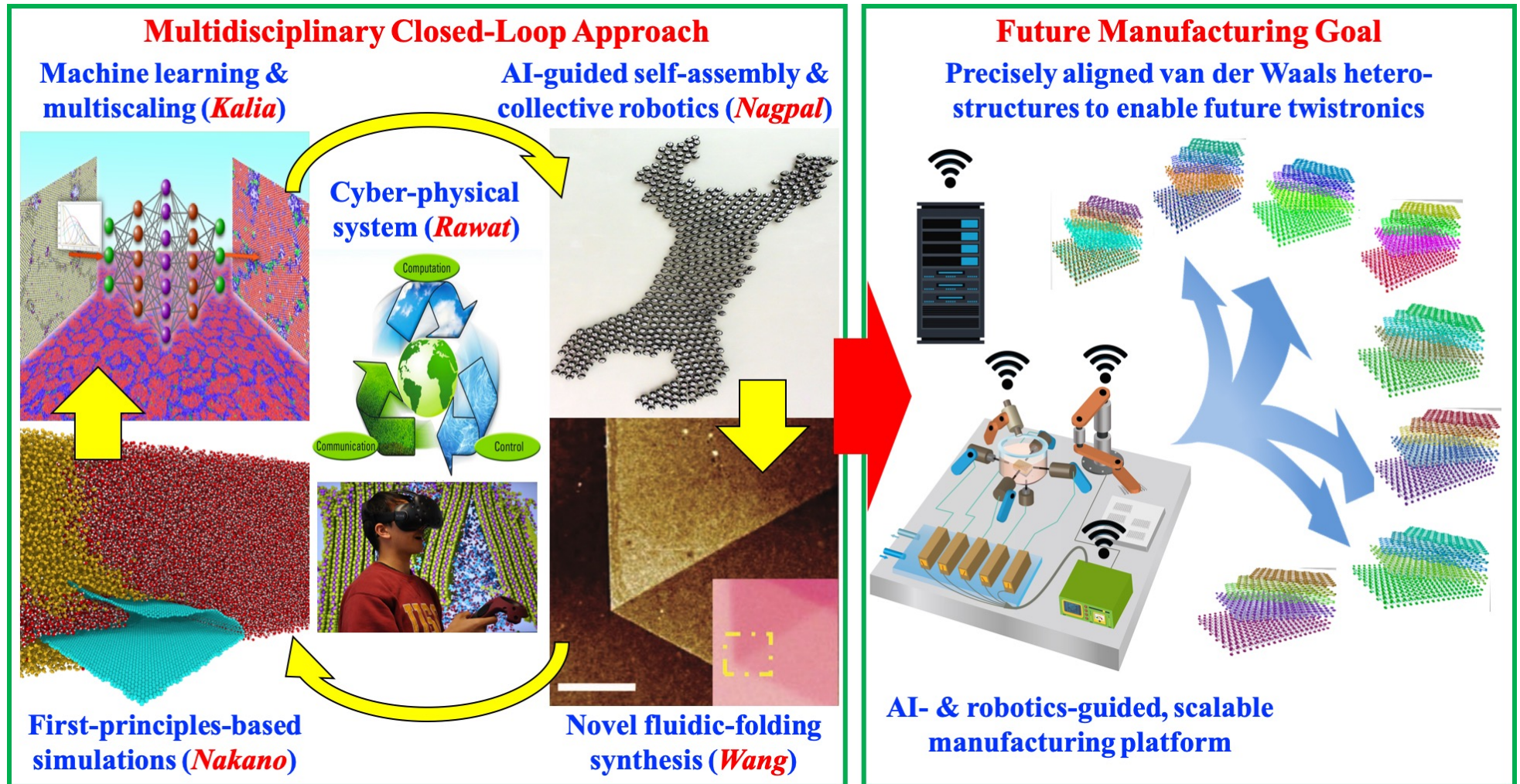
AIQ-XMaS Software Suite

AI & Quantum-Computing Enabled Exa Quantum Materials Simulator



USC-Howard Future Manufacturing

*FMRG: Artificial Intelligence Driven Cybermanufacturing
of Quantum Material Architectures*
\$3.75M NSF project (2020-2025)



Nagpal (Princeton); Kalia, Nakano, Wang (USC); Rawat (Howard)

Agenda: June 30 – July 2, 2022

Thursday, June 30, 2022		
Time (PDT)	Topic	Instructor
8:00 - 9:00 am	Introduction and logistics	Aiichiro Nakano
9:00 - 10:00 am	Molecular dynamics simulation basics	Priya Vashishta
10:00 - 11:00 am	Reactive molecular dynamics basics	Ken-ichi Nomura
11:00 am - 12:00 pm	Lunch break	
12:00 - 2:00 pm	Reactive molecular dynamics hands on: RXMD code	Ankit, Nitish, Pranab, Ruru
2:00 - 3:00 pm	Machine learning basics	Ken-ichi Nomura
Friday, July 1, 2022		
Time (PDT)	Topic	Instructor
8:00 - 9:00 am	Machine learning hands-on	Ankit, Nitish, Taufeq
9:00 - 10:00 am	Quantum molecular dynamics basics	Aiichiro Nakano
10:00 - 11:00 am	Quantum molecular dynamics hands-on: QXMD code (part 1)	Thomas Linker, Anikeya Aditya, Liqiu Yang
11:00 am - 12:00 pm	Lunch break	
12:00 - 1:00 pm	Quantum molecular dynamics hands-on: QXMD code (part 2)	Thomas Linker, Anikeya Aditya, Liqiu Yang
1:00 - 3:00 pm	Quantum computing basics and hands-on	Aiichiro, Shogo, Taufeq
Saturday, July 2, 2022		
Time (PDT)	Topic	Instructor
9:00 - 11:00 am	Participant presentations	All participants
11:00 - 11:15 am	Closing remarks	Pratibha Dev, Tao Wei

<https://cybermagics.netlify.app/workshop-schedule.html>

Logistics

- **Workshop courseware (lecture notes & Jupyter notebooks) is available at**
<https://cybermagics.netlify.app/workshop-resources.html>
- **Hands on training will use cloud resources**
 - 1. Google Colab (QXMD, RXMD, AI-machine learning)**
<https://colab.research.google.com>
 - 2. IBM Quantum (quantum computing)**
<https://quantum-computing.ibm.com>
- **Please ask questions any time during the lectures & hands-on sessions using Zoom chat**
- **Please prepare a one-slide self-introduction for Saturday (optional to observers)**
https://cybermagics.netlify.app/resources/CyberMAGICS_partipant_template.pptx