

QUANTUM MULTISCALE

Q-MS School 2024

Q-MS organizes schools on materials science based on first-principles multiscale modeling software. Comprehensive introductory lectures are followed by step-by-step training on materials modeling problems. More info and registration at www.quantum-multiscale.org/schools.html.

PROGRAM:

MONDAY JUNE 24: Fundamentals of Density

Functional Theory

TUESDAY JUNE 25: Advanced Functionals, Response

Properties, Non-Equilibrium

WEDNESDAY JUNE 26: Density Embedding and DFT

for Electrochemistry

THURSDAY JUNE 27: Continuum Models for

Solvents and Electrolytes in DFT

FRIDAY JUNE 28: Discrete Classical and Polarizable

Simulations for Solvent Effects

SCHOOL FORMAT: The school will focus on live lectures, tutorials, and student-driven project leveraging Python programs and open-source software, with a particular focus on: Quantum-ESPRESSO, ASE, QEpy, DFTpy, eDFTpy, Environ, LAMMPS, MBX.

REGISTRATION COSTS: The one-time registration fee (\$100) will cover all local expenses (food and lodging) for the whole duration of the school. Limited funding is available to support travel expenses.

FUNDING: We are grateful to the National Science Foundation Office of Advanced Cyberinfrastructure Award Numbers 2321102/2321103/23211042.

WHERE: Boise State University, Boise, Idaho 83725, USA.



WHEN: Check-in June 23 (from 3 PM).

Check-out June 28, 4 PM.

INSTRUCTORS:

Oliviero Andreussi (Boise State)

Md. Sharif Khan (Boise State)

Michele Pavanello (Rutgers)

Xuecheng Shao (Rutgers)

Xin Chen (Rutgers)

Jessica Martinez (Rutgers)

Valeria Rios Vargas (Rutgers)

Suman Saha (UC San Diego)

Iurii Timrov (PSI Zurich)

