

QUANTUM MULTISCALE

Q-MS School 2021

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 OCTOBER 11

08:00 AM: Fundamentals of DFT
09:30 AM: Simulations with QE
11:15 AM: Coffee Break
11:30 AM: **Seminar: D. Donadio**
12:30 PM: Lunch
01:30 PM: Post Processing for Materials Properties
03:00 PM: Advanced QE Simulations and PAOFLOW

TUESDAY OCTOBER 12

08:00 AM: Continuum Embedding
09:30 AM: Simulations with Environ
11:15 AM: Coffee Break
11:30 AM: **Seminar: B. Mennucci**
12:30 PM: Lunch
01:30 PM: Electrified Interfaces
03:00 PM: Advanced Environ Simulations

WEDNESDAY OCTOBER 13

08:00 AM: Quantum Embedding
10:00 AM: QE Simulations in Python
11:15 AM: Coffee Break
11:30 AM: **Seminar: L. Visscher**
12:30 PM: Lunch
01:30 PM: Density Embedding in QE
03:00 PM: Advanced Density Embedding Simulations
04:45 PM: Concluding Remarks

WHERE: The Lone Star Lodge and Marina
(www.lonestar-lodge.com) Pilot Point, Texas
76258, USA.



WHEN: Check-in October 10 (from 4 PM).
Check-out October 13, 5 PM.

INSTRUCTORS:

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