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:

Oliviero Andreussi (UNT)
Edan Bainglass (UNT)
Fernanda Bononi (UNT)
Marco Buongiorno Nardelli (UNT)
Davide Donadio (UC Davis)
Alessandro Genova (Kitware, Inc.)
Benedetta Mennucci (University of Pisa)
Michele Pavanello (Rutgers)
Xuecheng Shao (Rutgers)
Lucas Visscher (VU University Amsterdam)

FUNDING: We are grateful to Psi-k and the National Science Foundation for funding.

Information for virtual participants. Meetings will be live streamed via Zoom. A waiting room system is setup to only allow registered participants. Please be sure to have your full name displayed when trying to access the meetings. More details and materials related to the meetings and tutorials will be posted on the school website: http://www.quantum-multiscale.org/school-materials.html

MONDAY OCTOBER 11

08:00 AM Central Time (UTC-5:00) **Fundamentals of DFT**
Basic theory and algorithms of condensed-matter DFT
Instructor: D. Donadio
Meeting ID: 869 6391 8245

09:30 AM Central Time (UTC-5:00) **Simulations with QE**
Quantum Espresso for first-principles condensed-matter simulations of materials
Instructors: D. Donadio, F. Bononi
Meeting ID: 822 1641 2242

11:30 AM Central Time (UTC-5:00) **Seminar**
"Light-Matter Interactions in Aqueous Systems: Insights from Molecular Modeling"
Speaker: D. Donadio, University of California Davis
Meeting ID: 827 5436 0413

01:30 PM Central Time (UTC-5:00) **Post Processing for Materials Properties**
Theory and algorithms behind PAOFLOW
Instructors: M. Buongiorno Nardelli
Meeting ID: 827 5436 0413

03:00 PM Central Time (UTC-5:00) **Advanced QE Simulations and PAOFLOW**
Simulating properties of materials using PAOFLOW
Instructors: M. Buongiorno Nardelli, F. Cerasoli, A. Jayaraj
Meeting ID: 842 6576 6848

TUESDAY OCTOBER 12

08:00 AM Central Time (UTC-5:00) **Continuum Embedding**
Basic theory and algorithms of continuum models of solvent media in condensed-matter simulations
Instructors: O. Andreussi
Meeting ID: 846 9575 3296

09:30 AM Central Time (UTC-5:00) **Simulations with Environ**
Basic tutorials on using Environ with QE for solvation energies of molecules and materials
Instructors: O. Andreussi, E. Bainglass

Meeting ID: 891 4109 4681

11:30 AM Central Time (UTC-5:00) **Seminar**

"A quantum multiscale modeling of light-induced biological function: dream or reality?"

Speaker: Benedetta Mennucci, University of Pisa

Meeting ID: 869 1284 8573

01:30 PM Central Time (UTC-5:00) **Electrified Interfaces**

Models and algorithms of the electrochemical diffuse layer and computational electro-catalysis

Instructors: O. Andreussi

Meeting ID: 827 4380 7354

03:00 PM Central Time (UTC-5:00) **Advanced Environ Simulations**

Simulations of electrified interfaces and spectroscopies with Environ

Instructors: O. Andreussi, F. Bononi, E. Bainglass

Meeting ID: 896 8260 4340

WEDNESDAY OCTOBER 13

08:00 AM Central Time (UTC-5:00) **Quantum Embedding**

Basic theory and algorithms of subsystem DFT and quantum embedding methods

Instructors: M. Pavanello

Meeting ID: 873 5708 1573

10:00 AM Central Time (UTC-5:00) **QE Simulations in Python**

Run QE simulations through python using QEpy

Instructors: M. Pavanello, A. Genova

Meeting ID: 831 4147 7518

11:30 AM Central Time (UTC-5:00) **Seminar**

"Composite methods, Fragmentation and Embedding"

Speaker: Lucas Visscher, VU University Amsterdam

Meeting ID: 815 7008 6920

01:30 PM Central Time (UTC-5:00) **Density Embedding in QE**

Basic theory and algorithms of subsystem DFT as implemented in DFTpy and eDFTpy

Instructors: M. Pavanello

Meeting ID: 862 3474 3876

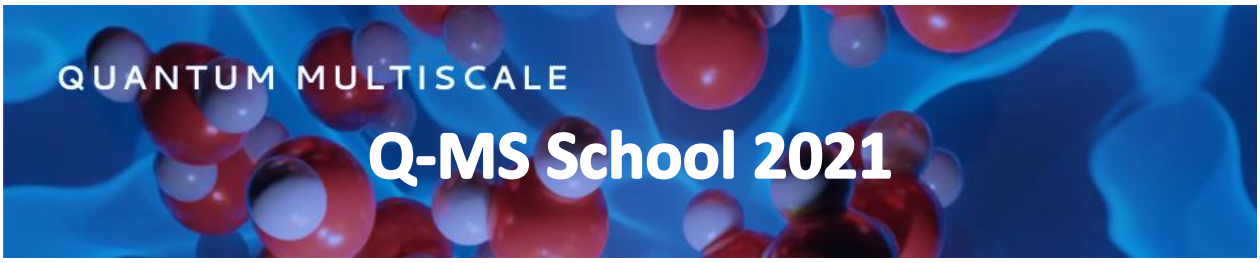
03:00 PM Central Time (UTC-5:00) **Advanced Density Embedding Simulations**

Simulations of subsystem DFT in python, using QEpy and eDFTpy

Instructors: M. Pavanello, A. Genova

Meeting ID: 868 9095 8031

FUNDING: We are grateful to Psi-k and the National Science Foundation for funding.



Meetings will be live streamed via Zoom. A waiting room system is setup, so please be sure to have your full name displayed when trying to access the meetings. More details related to the meetings and tutorials can be found on the school website: http://www.quantum-multiscale.org/schools.html

INVITED SEMINARS

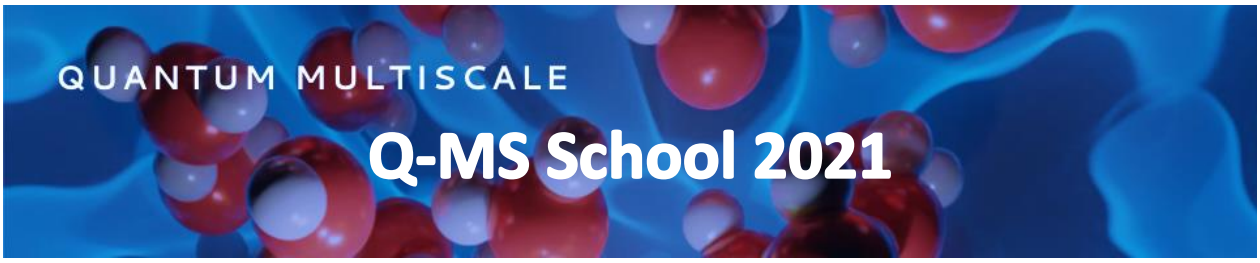
"Light-Matter Interactions in Aqueous Systems: Insights from Molecular Modeling"

Water is the universal solvent for environmental and biochemical reactions, and it is deeply interconnected with energy and food production. Despite their scientific and societal importance, we still have a shallow understanding of several key properties of water and aqueous systems. Hydrogen bonding dictates such properties, controlling an uncountable number of physicochemical phenomena, many of which shape the chemistry of our planet, and enable life as we know it. Electronic and vibrational spectroscopy has been deployed in various forms to investigate the elusive nature of hydrogen bonding in water and solutions. These techniques, however, provide indirect evidence of structural and dynamical motifs. Moreover, in the case of surfaces and interfaces, spectroscopic measurements are often hindered by limited sensitivity. Spectroscopy needs to be complemented by modeling, which can provide an insightful molecular interpretation of the experimental measurements.

In the first part of this lecture, I will illustrate the synergistic application of molecular modeling and ultrafast electron diffraction to unravel the relaxation dynamics of hydrogen bonds upon IR irradiation. Eventually, I will discuss the use of molecular simulations to interpret surface-sensitive vibrational spectroscopy investigations of the surface melting of ice. Finally, I will introduce a multiscale approach to compute the UV-visible light absorption of organic molecules solvated at the air-ice interface, and discuss the role of the ice surface in the photodegradation of pollutants in snowpacks.

Davide Donadio
Department of Chemistry,
University of California Davis
ddonadio@ucdavis.edu

Monday, Oct. 11
11:30 AM
Central Time (UTC-5:00)
Meeting ID: 869 1284 8573



Meetings will be live streamed via Zoom. A waiting room system is setup, so please be sure to have your full name displayed when trying to access the meetings. More details related to the meetings and tutorials can be found on the school website: http://www.quantum-multiscale.org/schools.html

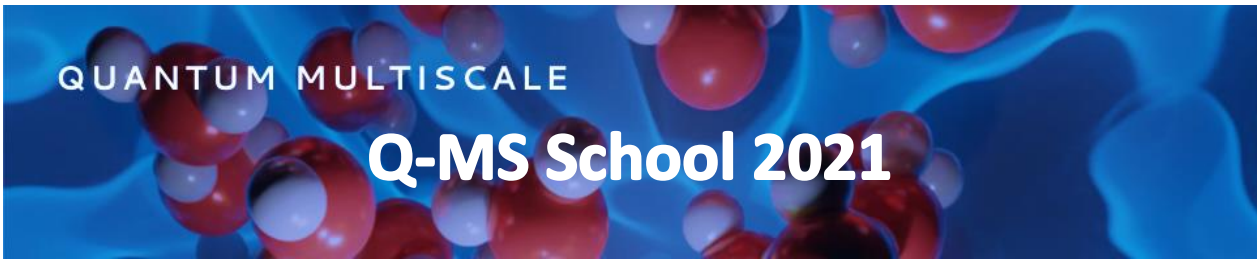
INVITED SEMINARS

"A quantum multiscale modeling of light-induced biological function: dream or reality?"

Organisms of all domains of life are capable of sensing, using and responding to light. The molecular mechanisms are diverse, but most commonly the starting event is an electronic excitation localized on a chromophoric unit bound to the protein matrix. The initial excitation rapidly "travels" across space and time finally leading to the protein conformational change required to complete the biological function. Here we discuss the main theoretical and methodological challenges of the modeling of such a multiscale problem, and we present possible strategies based on the integration of quantum chemistry and molecular dynamics.

Benedetta Mennucci
Department of Chemistry,
University of Pisa
Italy
benedetta.mennucci@unitpi.it

Tuesday, Oct. 12
11:30 AM
Central Time (UTC-5:00)
Meeting ID: 869 1284 8573



Meetings will be live streamed via Zoom. A waiting room system is setup, so please be sure to have your full name displayed when trying to access the meetings. More details related to the meetings and tutorials can be found on the school website: http://www.quantum-multiscale.org/schools.html

INVITED SEMINARS

"Composite methods, Fragmentation and Embedding"

In this seminar I want to discuss how different techniques of computational (quantum) chemistry can be combined in a single model. I will start by providing some examples of applications to illustrate, from a chemical or physical point of view, the advantages of a composite rather than a single quantum chemistry method. As methods also need efficient implementations, I will also look at developments in computer technology (massively parallel supercomputers, quantum computing) that should be considered when designing computational tools.

After this introduction, I will discuss how these concepts can be used with two of the major "workhorses" of quantum chemistry, Density Functional Theory (DFT) and Coupled Cluster Theory. I will discuss the theoretical foundation of the subsystem DFT (also known as Frozen Density Embedding) and the implementation and accuracy of composite methods that are based on this fragmentation. As an alternative that avoids use of kinetic energy functionals, I will furthermore introduce the alternative technique of localized orbital fragmentation.

Lucas Visscher
Department of Chemistry,
Vrije Universiteit Amsterdam
The Netherlands
l.visscher@vu.nl

Wednesday, Oct. 13
11:30 AM
Central Time (UTC-5:00)
Meeting ID: 815 7008 6920