

TSRC - Quantum Frontiers in Molecular Science (6/6/2022-6/10/2022)

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Updated: 5/19/22

Website <https://tinyurl.com/2p9cv4sd>

Slack Channel <https://tinyurl.com/4khfxrtv>

Meeting times: Meeting begins at 8 AM California (PDT) / 9 AM Telluride (MDT) / 11 AM New York (EDT) / 5 PM Brussels (GMT+2) / 11 PM China (GMT+8)
Meeting will be held throughout 6/6-6/10 from 9 to 11:30 AM MDT (Telluride, Colorado time zone).

Dynamics:

1. This will be a remote meeting run via Zoom. The virtual address will be shared by email with the participants.
2. There are 5 tutorial talks (40 min each) that will be uploaded in advance for everyone to watch asynchronously. The authors of these tutorials will also have 25 min allocated for a synchronous summary of the tutorial talk (10 min) followed by an open discussion (15 min).
3. All other talks will be held synchronously (20 min presentation + 5 min discussion).
4. There will be 1 min teasers of contributed presentations on Tuesday.
5. To enhance discussions during the sessions and beyond we have created a Slack channel. This will be the place to have the equivalent of hallway/bar/dinner/Colorado Ave. discussions.

PROGRAM

MONDAY 6/6

Analog Quantum Simulation

Chairs: Joel Yuen (UCSD) & Ignacio Franco (U. Rochester)

Tutorial Talk

Ivan Kassal (USydney)

Analog Quantum Simulation of Molecular Systems

8:45-9:00 MDT
9:00-9:25 MDT
9:25-9:50 MDT

Opening Remarks
Ivan Kassal (USydney)
Chang Woo Kim (ChonnamU)

Tutorial discussion
Analog Quantum Simulation of Open Quantum Systems

Open Quantum Systems

Chairs: Joel Yuen (UCSD) & Ignacio Franco (U. Rochester)

9:50-10:15 MDT
10:15-10:40 MDT
10:40-11:05 MDT

Nancy Makri (UIUC)
Doran Bennett (SMU)
Daniel Finkelstein-Shapiro (UNAM)

Real-time path integral simulations of excitation energy transfer in large molecular aggregates
Mesoscale quantum dynamics in molecular materials
Continuous transformations between non-Hermitian and dissipative dynamics
Capturing, predicting, and understanding optical signals: Harnessing machine learning to tackle energy dissipation in the condensed phase

11:05-11:30 MDT
11:30-12:00 MDT

Andrés Montoya-Castillo (CU Boulder)
Breakout/Slack Discussions

TUESDAY 6/7

Molecular Polaritonics

Chair: Justin Caram (UCLA)

Tutorial Talk

Wei Xiong (UCSD)

Ultrafast Dynamics of Molecular Vibrational Polaritons For Chemistry and Quantum Simulation

9:00-9:25 MDT
9:25-9:50 MDT
9:50-10:15 MDT
10:15-10:40 MDT
10:40-11:05 MDT

Wei Xiong (UCSD)
Jonathan Keeling (St Andrews)
Raphael Ribeiro (Emory)
Marissa Weichman (Princeton)
Ágnes Vibok (Debrecen)

Tutorial discussion
Modelling realistic open quantum systems: applications to molecular polaritons
Quantum energy diffusion in optical microcavities
Molecules in Optical Cavities: Precision Spectroscopy & Strong Light-Matter Interactions
Signature of a light-induced conical intersection in radiative emission from the lower polaritonic surface

11:05-11:30 MDT
11:30-12:00 MDT

1 min teasers
Breakout/Slack Discussions

Contributed Presentations (see list below)

WEDNESDAY 6/8

Quantum information

Chair: Raphael Ribeiro (Emory)

Tutorial Talk

Artur Izmaylov (UToronto)

Quantum Computing Approaches for the Electronic Structure Problem

9:00-9:25 MDT
9:25-9:50 MDT
9:50-10:15 MDT

Artur Izmaylov (UToronto)
Sabre Kais (Purdue)
Ben Sussman (NRC/Ottawa)

Tutorial discussion
Quantum Machine Learning for Complex Chemical Systems on Quantum Devices
Ultrafast Quantum Sensing: From Ranging to 3D Scene Reconstruction

Molecular Spectroscopy

Chair: Raphael Ribeiro (Emory)

10:15-10:40 MDT
10:40-11:05 MDT
11:05-11:30 MDT
11:30-12:00 MDT

Justin Caram (UCLA)
Ulrich Kleinekathoefer (Bremen)
Greg Engel (UChicago)
Breakout/Slack Discussions

Design principles for highly diagonal molecular transitions and ultranarrow linewidths
Multi-scale modelling of spectral densities and absorption spectra from different light-harvesting complexes
TBA

THURSDAY 6/9

Chirality in Light Matter Interactions

Chair: Bing Gu (UCI/Westlake)

Tutorial Talk

Olga Smirnova (MBI)

Geometric magnetism and new enantio-sensitive observables in photoionization of chiral molecules

9:00-9:25 MDT
9:25-9:50 MDT
9:50-10:15 MDT
10:15-10:40 MDT

Olga Smirnova (MBI)
Melanie Schnell (DESY/UKiel)
Hendrike Braun (UKassel)
Joel Yuen-Zhou (UC San Diego)

Tutorial discussion
Coherent microwave excitations for enantiomer-selective population transfer in chiral molecules
Circular dichroism in the ion yield of chiral molecules
Unconventional nonlinear light-matter interactions

Quantum Control with Few Cycle Lasers

Chair: Bing Gu (UCI/Westlake)

10:40-11:05 MDT
11:05-11:30 MDT
11:30-12:00 MDT

Tyler Coker (Michigan State U)
Christian Heide (SLAC/Stanford)
Breakout/Slack Discussions

Lightwave-driven scanning tunneling spectroscopy on the atomic scale
Light-field driven electron dynamics in solids

FRIDAY 6/10

Emerging Motifs in Quantum Control

Chair: Marissa Weichman (Princeton)

Tutorial Talk

Prineha Narang (Harvard/UCLA)

Cavity control of nonlinearities in molecular matter

9:00-9:25 MDT
9:25-9:50 MDT
9:50-10:15 MDT
10:15-10:40 MDT
10:40-11:05 MDT
11:05-11:30 MDT
11:30-12:00 MDT

Prineha Narang (Harvard/UCLA)
Jianshu Cao (MIT)
Ignacio Franco (Rochester)
Bing Gu (UCI/Westlake)
Paul Brumer (UToronto)
Overall Discussion
Zoom Beer Hour

Tutorial discussion
Emerging Phenomena in Light-matter Interactions
Light field control of real and virtual charge carriers
Control of quantum interference in molecular two-photon absorption by entangled light
Quantum Control of Scattering at Cold and Ultracold Temperatures