

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

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Updated: 6/8/22

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

Slack Channel <https://tinyurl.com/bdcv6ekn>

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

Wei Xiong (UCSD)
Jonathan Keeling (St Andrews)

Tutorial discussion
Modelling realistic open quantum systems: applications to molecular polaritons

9:50-10:15 MDT Raphael Ribeiro (Emory) Quantum energy diffusion in optical microcavities
10:15-10:40 MDT Marissa Weichman (Princeton) Molecules in Optical Cavities: Precision Spectroscopy & Strong Light-Matter Interactions
10:40-11:05 MDT Ágnes Vibok (Debrecen) Signature of a light-induced conical intersection in radiative emission from the lower polaritonic surface

11:05-11:30 MDT 1 min teasers Contributed Presentations (see list below)
11:30-12:00 MDT Breakout/Slack Discussions

WEDNESDAY 6/8

Tutorial Talk

Quantum information

Chair: Raphael Ribeiro (Emory)

Artur Izmaylov (UToronto)

Quantum Computing Approaches for the Electronic Structure Problem

9:00-9:25 MDT Artur Izmaylov (UToronto) Tutorial discussion
9:25-9:50 MDT Sabre Kais (Purdue) Quantum Machine Learning for Complex Chemical Systems on Quantum Devices
9:50-10:15 MDT Ben Sussman (NRC/Ottawa) Ultrafast Quantum Sensing: From Ranging to 3D Scene Reconstruction

Molecular Spectroscopy

Chair: Raphael Ribeiro (Emory)

10:15-10:40 MDT Justin Caram (UCLA) Design principles for highly diagonal molecular transitions and ultranarrow linewidths

10:40-11:05 MDT Ulrich Kleinekathoefer (Bremen) Multi-scale modelling of spectral densities and absorption spectra from different light-harvesting complexes
11:05-11:30 MDT Greg Engel (UChicago) Ultrafast excitonic exchange between valleys in monolayer MoS₂ limits optical valleytronic applications
11:30-12:00 MDT Breakout/Slack Discussions

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 Olga Smirnova (MBI) Tutorial discussion
9:25-9:50 MDT Melanie Schnell (DESY/UKiel) Coherent microwave excitations for enantiomer-selective population transfer in chiral molecules
9:50-10:15 MDT Hendrike Braun (UKassel) Circular dichroism in the ion yield of chiral molecules
10:15-10:40 MDT Joel Yuen-Zhou (UC San Diego) Unconventional nonlinear light-matter interactions

Quantum Control with Few Cycle Lasers

Chair: Bing Gu (UCI/Westlake)

10:40-11:05 MDT Tyler Coker (Michigan State U) Lightwave-driven scanning tunneling spectroscopy on the atomic scale
11:05-11:30 MDT Christian Heide (SLAC/Stanford) Light-field driven electron dynamics in solids
11:30-12:00 MDT Breakout/Slack Discussions

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	Prineha Narang (Harvard/UCLA)	Tutorial discussion
9:25-9:50 MDT	Jianshu Cao (MIT)	Emerging Phenomena in Light-matter Interactions
9:50-10:15 MDT	Ignacio Franco (Rochester)	Light field control of real and virtual charge carriers
10:15-10:40 MDT	Bing Gu (UCI/Westlake)	Control of quantum interference in molecular two-photon absorption by entangled light
10:40-11:05 MDT	Paul Brumer (UToronto)	Quantum Control of Scattering at Cold and Ultracold Temperatures
11:05-11:30 MDT	Overall Discussion	
11:30-12:00 MDT	Zoom Beer Hour	

Presentation Order

Contributed Presentations

1 Leonardo Calderon (Toronto)	Nonadiabatic sunlight harvesting
2 Singh Davinder (Toronto)	Dissipation, flux and fluctuations in a driven open quantum system
3 Claire Dickerson (UCLA)	Designing and Predicting Ultranarrow Yb(III) Molecular Transitions
4 Piper Fowler-Wright (St. Andrews)	Efficient many-body non-Markovian dynamics of organic polaritons
5 Antonio Garzón (Rochester/McGill)	The Stark Control of Electrons at Interfaces (SCELI)
6 Zixuan (Andrew) Hu (Purdue)	The quantum condition space
7 Arghadip Koner (UCSD)	High precision measurements using cavity enhanced backaction evading Raman spectroscopy
8 Kai Liu (Duke)	Improved Efficiency of Open Quantum System Simulations Using Matrix Products States in the Interaction Picture
9 Nicola Mayer (MBI)	Control of achiral and chiral media using synthetic chiral light
10 Federico Mellini (UCSD)	The role of dark states in energy transfer dynamics between entangled molecules
11 Masato Morita (Toronto)	Quantum scattering calculation for the cold and ultracold $\text{Li}(2S) + \text{LiNa}(a3\Sigma^+) \rightarrow \text{Li}_2(a3\Sigma^+) + \text{Na}(2S)$ reaction
12 Sindhana Pannir-Sivajothi (UCSD)	Driving chemical reactions with polariton condensates
13 Kai Schwennicke (UCSD)	Enantioselective Topological Frequency Conversion
14 Philipp Stegmann (MIT)	Quantum Corrections in the Higher-Order Photon Counting Statistics
15 Vishal Tiwari (Rochester)	Floquet engineering optical properties of solids
16 Otabek Umarov (Debrecen)	Topological aspects of light-induced degeneracies in polyatomic molecules
17 Manas Sajjan (Purdue)	Quantum machine learning for materials and molecules
18 Adrien Devolder (Toronto)	Coherent control of total cross section: Coherent optical theorem
19 Tengting Chen (UCSD)	Cavity-Enabled Enhancement of Ultrafast Intramolecular Vibrational Redistribution over Pseudorotation