

Final Technical Report

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Grantee Name: Board of Regents, NSHE obo University of Nevada, Reno

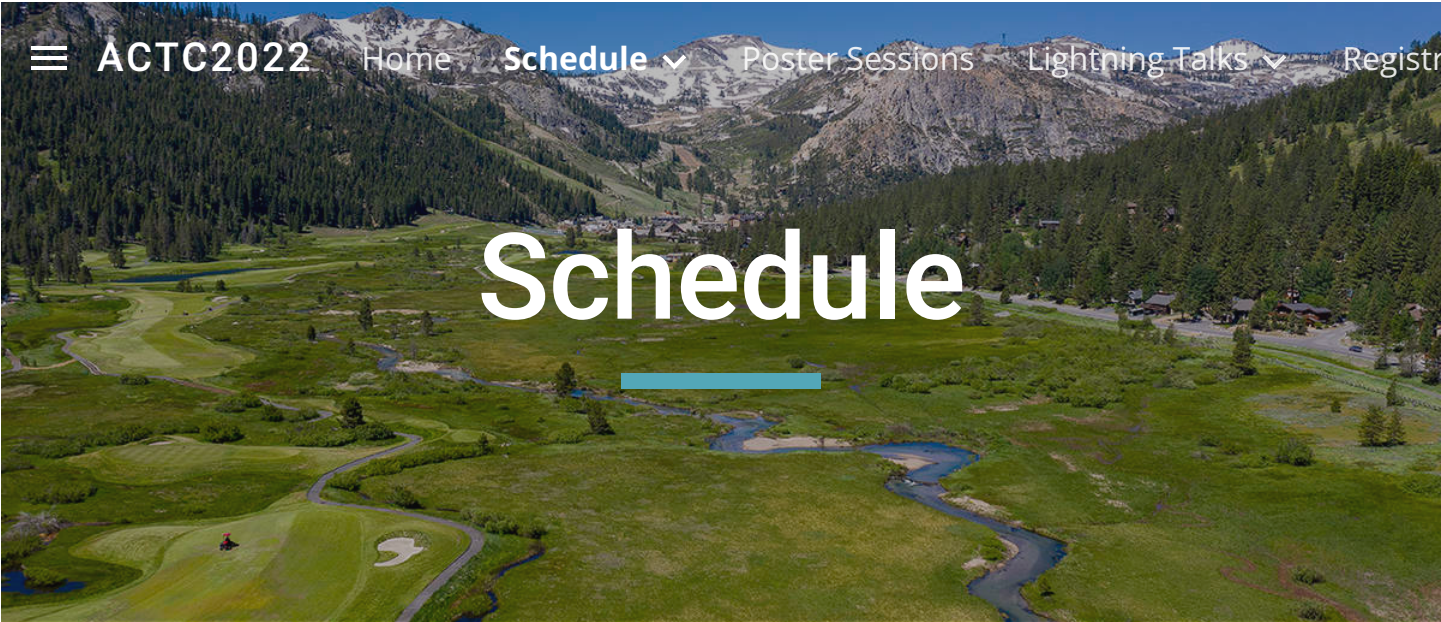
Title: Support for the American Conference on Theoretical Chemistry 2022

Period of Performance: 06/01/2022 – 05/31/2023

PI: Sergey A. Varganov

The 2022 American Conference on Theoretical Chemistry (ACTC) took place July 25 – July 28 at The Village at Palisades Tahoe in Palisades Tahoe, California (formerly Squaw Valley). The Chair and Vice-Chair of the conference were Todd Martínez (SLAC National Accelerator Laboratory) and David Beratan (Duke University), respectively, and the Deputy Chairs and Local Organizers were Edward Hohenstein (SLAC National Accelerator Laboratory) and Sergey Varganov (University of Nevada, Reno). Held every three years since 1972, the ACTC plays a vital role in presenting pioneering research to a diverse audience in theoretical and computational chemistry. The ACTC 2022 brought together 27 invited speakers who are at the forefront of the field (see conference program below), and provided opportunities for about 150 junior scientists and graduate students to present their work in poster format and exchange ideas with leaders in the field.

The funds provided by this DOE award were used to defray \$100 of the registration costs for the first registered 98 graduate students and postdoctoral scholars attending the conference (see list of students below). The DOE support was acknowledged on the ACTC 2022 web page (<https://sites.google.com/view/actc2022/home>) and on a slide that was shown during Conference Introduction and breaks between talks.



The conference will run from Monday, July 25, through Thursday, July 28. Attendees should plan to arrive and register on Sunday evening and leave on Thursday evening or Friday. Plenary sessions will begin on Monday at 9:00 a.m. in the Events Center and end Thursday at 3:00 p.m. A complete schedule can be found below.

ACTC will provide attendees with a continental breakfast on each day of the conference as well as lunch on M, T, and Th. Breakfast will be served on the deck adjoining the Events Center, and lunch will be served on the KT Deck shown in red on [this property map](#). On Wednesday, attendees will have the entire afternoon free to [explore the beautiful surroundings](#).

On Tuesday evening after the poster session, enjoy [the blues at a free outdoor concert](#). On Wednesday afternoon before the banquet, participate in a [free yoga class on the plaza](#). And on Thursday evening, it's the Auld Dubliner restaurant's turn to host a family-friendly [free bingo night](#).

[PDF Booklet of Talk Abstracts](#)

SUNDAY, JULY 24

TIME

5:00-7:00 pm	REGISTRATION (near the front desk of the Palisades)
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MONDAY, JULY 25

TIME

SPEAKER

8:00-9:00 am	Breakfast and late registration
8:50-9:00am	Welcome: Todd Martinez
	Morning Session Chair: Tom Markland, Stanford University
9:00-9:35am	Sharon Hammes-Schiffer, Yale University Photoinduced Proton-Coupled Electron and Energy Transfer
9:35-10:10am	David Beratan, Duke How does biology bifurcate electrons with high efficiency?
10:10-10:40am	Rising Talent: Lisa Fredin, Lehigh University Predicting Effects of Dynamic Disorder in Molecular Semiconductors
10:40-11:00am	BREAK
11:00-11:35am	Neepta Maitra, Rutgers University at Newark Recent developments in the exact factorization approach to coupled

dynamics

11:35-12:10pm	Katherine Hunt, Michigan State University Nonadiabatic transition probabilities in transient electric fields
12:10-1:30pm	LUNCH Afternoon Session Chair: Ben Levine, Stony Brook University
1:30-2:05pm	Artur Izmaylov, University of Toronto Algebraic techniques for quantum chemistry on a quantum computer
2:05-2:25pm	Promoted Lightning Talk – Maristella Alessio, USC Equation-of-Motion Coupled-Cluster Protocol for Computing Molecular Magnetic Properties
2:25-2:45pm	Promoted Lightning Talk – Mariya Romanova, UC Santa Barbara Stochastic cRPA calculations of screened interactions in graphene Moire states at high pressures
2:45-3:05pm	BREAK
3:05-3:40pm	Rick Heller, Harvard University The momentum of models: Keys to the high-Tc superconductors
3:40-4:15pm	Dominika Zgid, University of Michigan Green's function embedding methods for solids
4:30-6:30pm	Poster Session (Posters #1-78)

TUESDAY, JULY 26

TIME	SPEAKER
8:00-9:00	Breakfast Morning Session Chair: Joseph Subotnik, Penn
9:00-9:35am	David Masiello, U of Washington Probing Infrared- to Optical-Frequency Responses in Plasmonic and Photonic Nanostructures with Fast Electron Spectroscopy
9:35-10:10am	Eran Rabani, UC Berkeley Modeling the dynamics of excitons and multiexcitons in semiconductor nanostructures
10:10-10:40am	Rising Talent: Yuan Ping, UC Santa Cruz Ab-initio Spin Dynamics in Solids
10:40-11:00am	BREAK
11:00-11:35 pm	Christine Aikens, Kansas State University

Photoluminescence: Applications and Development

11:35-12:10pm	Baron Peters, UIUC Modeling the kinetics of antifreeze protein adsorption: Buffon's needle at the nanoscale
12:10-1:30	LUNCH Afternoon Session Chair: Christoph Bannwarth, RWTH Aachen
1:30-2:05pm	Martin Head-Gordon, UC Berkeley Density functional theory for simulating core spectroscopy: Problems, solutions and applications.
2:05-2:25pm	Promoted Lightning Talk – Alex Mironenko, UIUC Non-empirical Tight Binding Theory
2:25-2:45pm	Promoted Lightning Talk – Jacqueline Shea, Stanford Active Space Control in State Averaged CASSCF Methods
2:45-3:05pm	BREAK
3:05-3:40pm	Annabella Selloni, Princeton University Water-Titania Interfaces from Ab Initio Deep Neural Network Simulations
3:40-4:15pm	Piotr Piecuch, Michigan State University Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected-CI-Driven Coupled-Cluster Computations
4:30-6:30pm	Poster Session (Posters #79-156)

WEDNESDAY, JULY 27

TIME	SPEAKER
8:00-9:00am	Breakfast Morning Session Chair: David Limmer, UC Berkeley
9:00-9:35am	Mark Tuckerman, New York University Topology, Molecular Simulation, and Machine Learning as tools to explore Structure and Phase Behavior in Molecular and Atomic Crystals
9:35-10:10am	Marivi Fernandez-Serra, Stony Brook University Machine learning approaches to improve the exchange and correlation functional in DFT
10:10-10:40am	Rising Talent: Pratyush Tiwary, University of Maryland From atoms to mechanisms: AI augmented chemistry for molecular simulations and beyond



10:40-11:00am	BREAK
11:00-11:35am	Olga Dudko, UC San Diego Universality vs. Specificity in Synaptic Transmission
11:35-12:10pm	Suri Vaikuntanathan, University of Chicago Enhanced associative memory, classification and learning with active dynamics
12:10-6:00pm	LUNCH ON YOUR OWN + Free Time
5:30-9:00pm	Aerial Tram to High Camp
6:00-9:00pm	Conference Banquet in the Terrace Room. Tickets required.
6:00-7:00pm	Happy Hour with music
7:00-9:00pm	Dinner

THURSDAY, JULY 28

TIME	SPEAKER
8:00 – 9:00am	Breakfast
	Morning Session Chair: Alice Walker, Wayne State University
9:00-9:35am	Valeria Molinero, University of Utah Modeling anion exchange membranes for fuel cells
9:35-10:10am	Rigoberto Hernandez, Johns Hopkins University Spiral feedback between computation and experiment at the nano-bio interface
10:10-10:40am	David Mobley, UC Irvine An update on the Open Force Field Initiative: Progress, Plans and Opportunities
10:40-11:00am	BREAK
11:00-11:30am	Rising Talent: Matthias Heyden, Arizona State University Anharmonic Vibrational Dynamics in Complex Molecular Systems
11:30-11:50am	Promoted Lightning Talk – Yang Yang, UW Madison Incorporating Nuclear Quantum Effects in ab initio Molecular Dynamics
11:50-12:10pm	Promoted Lightning Talk – Tim Zuehlsdorff, Oregon State University Beyond the Condon approximation: Modeling linear optical spectra using molecular dynamics simulations
12:10-1:30pm	LUNCH

Afternoon Session Chair: Fang Liu, Emory University

- 1:30-2:05pm Sergey Varganov, University of Nevada at Reno
Spin Relaxation in Lanthanide-Based Single-Ion Magnets
- 2:05-2:40pm Tom Markland, Stanford
Imaging and elucidating molecular orientational structure and
dynamics in solution with optically induced anisotropy in time-resolved
scattering
- 2:40 END
- 3:30 Optional Hike - [Shirley Canyon](#)

Confirmed Speakers:

Christine Aikens, Kansas State University

David Beratan, Duke University

Olga Dudko, University of California, San Diego

Marivi Fernandez-Serra, State University of New York, Stony Brook

Sharon Hammes-Schiffer, Yale University

Martin Head-Gordon, University of California, Berkeley

Eric Heller, Harvard University

Rigoberto Hernandez, Johns Hopkins University

Katharine Hunt, Michigan State University

Artur Izmaylov, University of Toronto

Neepta Maitra, Hunter College

Tom Markland, Stanford University

David Masiello, University of Washington

David Mobley, University of California, Irvine

Valeria Molinero, University of Utah

Baron Peters, University of Illinois, Urbana-Champaign

Piotr Piecuch, Michigan State University

Eran Rabani, University of California, Berkeley

Annabella Selloni, Princeton University

Mark Tuckerman, New York University

Suri Vaikuntanathan, University of Chicago

Sergey Varganov, University of Nevada, Reno

Dominika Zgid, University of Michigan

Rising Talent Speakers:

Lisa Fredin, Lehigh University

Matthias Heyden, Arizona State University

Pratyush Tiwary, University of Maryland

Yuan Ping, University of California, Santa Cruz

LIST OF GRADUATE STUDENTS AND POSTDOCTORAL SCHOLARS

1	Abdulrahman	46	Jiri Suchan	90	Yanze Wu
	Aldossary	47	Johannes Reiff	91	Yinan Shu
2	Abhishek Mitra	48	John Weber	92	Yorick Lassmann
3	Adam Rettig	49	Jonathan Wong	93	Yuezhi Mao
4	Alec Wills	50	Joseph Kelly	94	Yuming Shi
5	Amiel Stephen Paz	51	Junhan Chen	95	Zehua Chen
6	Andrew Durden	52	Katherine Kidder	96	Zeke Piskulich
7	Anthony Mannino	53	Kejun Li	97	Zeyu Zhou
8	Anthony Poggioli	54	Kelsey Parker	98	Zhenling Wang
9	Antonio Prlj	55	Ken Miyazaki		
10	Ariel Gale	56	Kevin Carter-Fenk		
11	Arshad Mehmood	57	Kiriko Terai		
12	Becky Hanscam	58	Kye Hunter		
13	Benjamin Rousseau	59	Leonardo dos Anjos		
14	Bokang Hou		Cunha		
15	Brandon Neff	60	Leopoldo Mejia		
16	Caitlin Hetherington	61	Maristella Alessio		
17	Cheng-Han Li	62	Mark Hix		
18	Christian Seitz	63	Mary Kate Caucci		
19	Christopher Malbon	64	Maureen Kitheka		
20	Claire Dickerson	65	Michael Chen		
21	Daniel Chabeda	66	Michael Sauer		
22	Daniel King	67	Nadine Bradbury		
23	Daniel Weinberg	68	Nathan London		
24	Daria Nakritskaia	69	Nathan Zimmerberg		
25	Dayana Bashirova	70	Ningyi Lyu		
26	Diptarka Hait	71	Nuong Nguyen		
27	Dipti Jasrasaria	72	Patricia Poths		
28	Donghwan Kim	73	Paul Robinson		
29	Eugen Hruska	74	Phillips Hutchison		
30	Evaristo Villaseco	75	Praveen Ranganath		
31	Fangchun Liang		Prabhakar		
32	Fangning Ren	76	Ruhee Dcunha		
33	Gautam Stroschio	77	Ryan Szukalo		
34	Guorong Weng	78	Shawn Opfer		
35	Hengyuan Shen	79	Sourav Dey		
36	Humanath Poudel	80	Sutirtha Chowdhury		
37	Ilker Deveci	81	Thomas Fay		
38	Ilya Dergachev	82	Tian Qiu		
39	Jackson Elowitz	83	Tommy (Kailai) Lin		
40	Jacob Hirschi	84	Vishikh Athavale		
41	Jacob Sivak	85	Vsevolod Dergachev		
42	Jesus Valdiviezo	86	Wook Shin		
43	Jiashu Liang	87	Xuechen Zheng		
44	Jiayun Zhong	88	Xuelan Wen		
45	Jie Bao	89	Xuezhi Bian		