

	Monday	Tuesday	Wednesday	Thursday	Friday	
9:00	Discussion Leader: J. S. Tse 9:00 Opening remarks, followed by Compute Canada presentation by R. K. Bowles	Discussion Leader: J. W. Hollett 9:00 Marco A. C. Nascimento <i>Quantum Interference and the Nature of the Chemical Bond</i>	Free time	Discussion Leader: A. J. Thakkar 9:00 T. Daniel Crawford <i>Reduced Scaling Coupled Cluster Linear Response Theory</i>	Discussion Leader: A. L. L. East 9:00 Neil S. Ostlund <i>Applying the Semantic Web to Quantum Chemistry</i>	
9:40	9:40 George C. Schatz <i>Self-assembled plasmonic structures</i>	9:40 Raymond A. Poirier <i>Molecular Density and Radial density: Properties of Atoms and Bonds in Molecules</i>		9:40 Paul W. Ayers <i>Learning New, and Old, Chemical Concepts from Data</i>	9:40 Matt I. J. Probert <i>Quantum Dynamics of Hydrogen</i>	
10:20	10:20 Coffee break	10:20 Coffee break		10:20 Coffee break	10:20 Coffee break	
10:50	Discussion Leader: E. R. Johnson 10:50 Josef W. Zwanziger <i>Photoelasticity of glass</i>	Discussion Leader: R. Fournier 10:50 Erin R. Johnson <i>Dispersion-corrected DFT for Molecular Crystals and Polymorphism</i>		Discussion Leader: M. E. Mandy 10:50 Styliani Consta <i>Star morphologies of charged droplets beyond Rayleigh limit</i>	Discussion Leader: R. K. Bowles 10:50 Ivan Saika-Voivod <i>Inspiration from water: melting by cooling and the freezing of nanodroplets</i>	
11:30	11:30 Irina Paci <i>Optical and dielectric properties of metal/polymer nanocomposites</i>	11:30 Georg Schreckenbach <i>Modelling of one- and two-dimensional systems: mineral surfaces, interfaces, polymers, two-dimensional materials</i>		11:30 James T. Kindt <i>Breaking the law of mass action: analyzing aggregation statistics from unbiased simulations of small systems</i>	11:30 Tom K. Woo <i>Materialsinformatics: Datamining and Machine Learning Recognition of High Performance Materials for Carbon Capture</i>	
12:10	Lunch break (catered)	Lunch break (catered)		12:50 CATC Honourary Lecture Introduction: Dennis Salahub Arvi Rauk <i>From Small Molecules to Large: Twists and Turns</i>	Lunch break (catered)	Lunch break (catered)
1:10		Discussion Leader: A. L. L. East 1:10 Michael S. Schuurman <i>Substituent Effects on Dynamics at Conical Intersections</i>			Discussion Leader: R. Z. Khaliullin 1:10 Axel D. Becke <i>Tests of a new approach to excited-state energy computations</i>	Discussion Leader: R. C. Mawhinney 1:10 Hiromi Nakai <i>Harmonic Solvation Model (HSM) to Evaluate Condensed-Phase Thermochemistry</i>
1:50	Discussion Leader: P. G. Kusalik 1:50 Dennis R. Salahub <i>Multiscale Modeling of Chemical Reactions in Complex Environments</i>	1:50 Ajit J. Thakkar <i>Why and how should constrained dipole oscillator strength distributions be constructed?</i>		Discussion Leader: A. Brown 1:50 Mark Thachuk <i>Description and Control of Dissociation Channels in Gas-Phase Protein Complexes</i>	1:50 Viktor N. Staroverov <i>Origin of the step structure of molecular exchange-correlation potentials</i>	1:50 Jeremy Schofield <i>Simple microscopic models of complex systems</i>
2:30	2:30 Andriy Kovalenko <i>[cancelled – no show]</i> <i>[Dennis Salahub continued his talk after the ~ 20 minute power outage]</i>	2:30 T. Seideman Sai Ramakrishna <i>Current-driven dynamics in molecular-scale electronics [Sai is Tamar's research associate]</i>		2:30 Ronald M. Levy <i>Exploring Free Energy and Fitness Landscapes of Proteins for Molecular Recognition, Binding, and Allostery</i>	2:30 Poster session B	2:30 Mark E. Tuckerman <i>Exploration and generation of free energy landscapes of molecular crystals and oligopeptides</i>
3:10	3:10 Coffee break	3:10 Poster Session A		3:10 Coffee break		3:10 Radu Iftimie <i>Donor-Bridge-Acceptor Proton Transfer in Aqueous Solution</i>
3:40	Discussion Leader: G. H. Peslherbe 3:40 Stephen J. Klippenstein <i>From Theoretical Reaction Dynamics to Combustion Modeling</i>		Discussion Leader: C. C. Pye 3:40 Dvira Segal Rene Fournier <i>Global optimization-density functional theory study of tin oxide clusters</i>	3:50 Afterparty at the Owl (campus pub) (cash bar)		
4:20	4:20 Ahren W. Jasper <i>Multistate trajectory and statistical theories of spin-forbidden kinetics</i>		4:20 Hiromi Nakai <i>[postponed to Friday 1:10 due to illness]</i> <i>[replaced by two 20-minute bonus talks by Ron Levy and Mark Tuckerman]</i>			

5:00

7:00-10:00
Sunday Reception & Registration

7:00 Banquet, DoubleTree Hilton ~ 8:00 banquet speaker: Raymond Francis, NASA Jet Propulsion Laboratory
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CSTCC2016, July 10-15, University of Regina