



CSTCC2016

27th Canadian Symposium on Theoretical and Computational Chemistry

July 10-15, 2016
University of Regina
Regina, Saskatchewan

Confirmed speakers (updated March 2, 2016):

Paul Ayers, McMaster University, Canada
Axel Becke, Dalhousie University, Canada
Styliani Conostas, University of Western Ontario, Canada
T. Daniel Crawford, Virginia Tech University, USA
Radu Iftimie, University of Montreal, Canada
Ahren W. Jasper, Sandia National Labs, USA
Erin Johnson, Dalhousie University, Canada
James T. Kindt, Emory University, USA
Steven J. Klippenstein, Argonne National Labs, USA
Andriy Kovalenko, National Research Council, Canada
Ronald M. Levy, Temple University, USA
Hiromi Nakai, Waseda University, Japan
Marco A. C. Nascimento, U. Federale Rio de Janeiro, Brazil

Neil S. Ostlund, Chemical Semantics, Inc., USA
Irina Paci, University of Victoria, Canada
Ray Poirier, Memorial University, Canada
Matthew I. J. Probert, University of York, U.K.
Arvi Rauk, University of Calgary, Canada
Ivan Saika-Voivod, Memorial University, Canada
Dennis Salahub, University of Calgary, Canada
George C. Schatz, Northwestern University, USA
Jeremy Schofield, University of Toronto, Canada
Georg Schreckenbach, University of Manitoba, Canada
Michael Schuurman, National Research Council, Canada
Dvira Segal, University of Toronto, Canada
Tamar Seideman, Northwestern University, USA
Viktor Staroverov, University of Western Ontario, Canada
Mark Thachuk, University of British Columbia, Canada
Ajit Thakkar, University of New Brunswick, Canada
Mark E. Tuckerman, New York University, USA
Tom Woo, University of Ottawa, Canada
Josef Zwanziger, Dalhousie University, Canada

Last modified April 18, 2016 (AE)

	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>	4:00 CATC Annual General Meeting		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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