The 33rd Annual

Symposium

On

Chemical Physics

at the

University of Waterloo

November 3-5, 2017

Acknowledgements

We are very grateful to the following sponsors
for their generous financial support of this conference.

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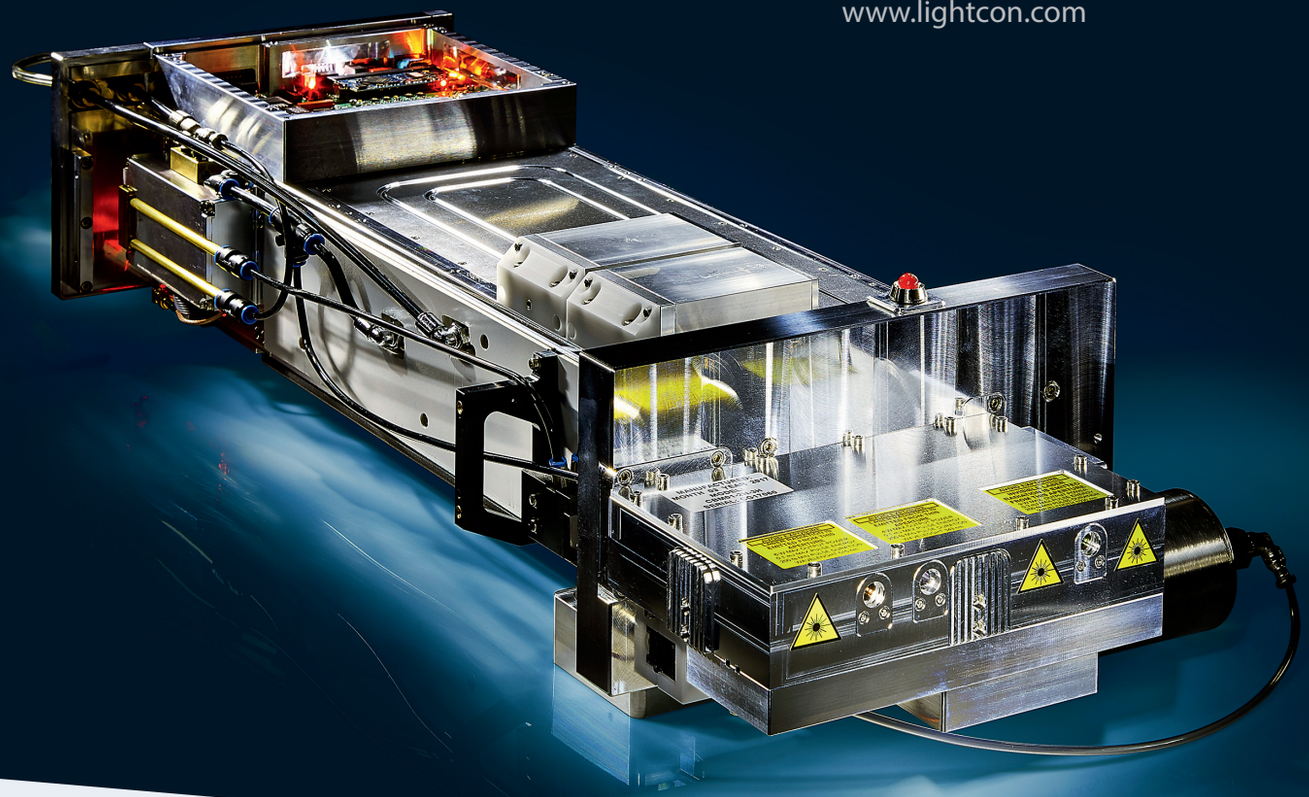

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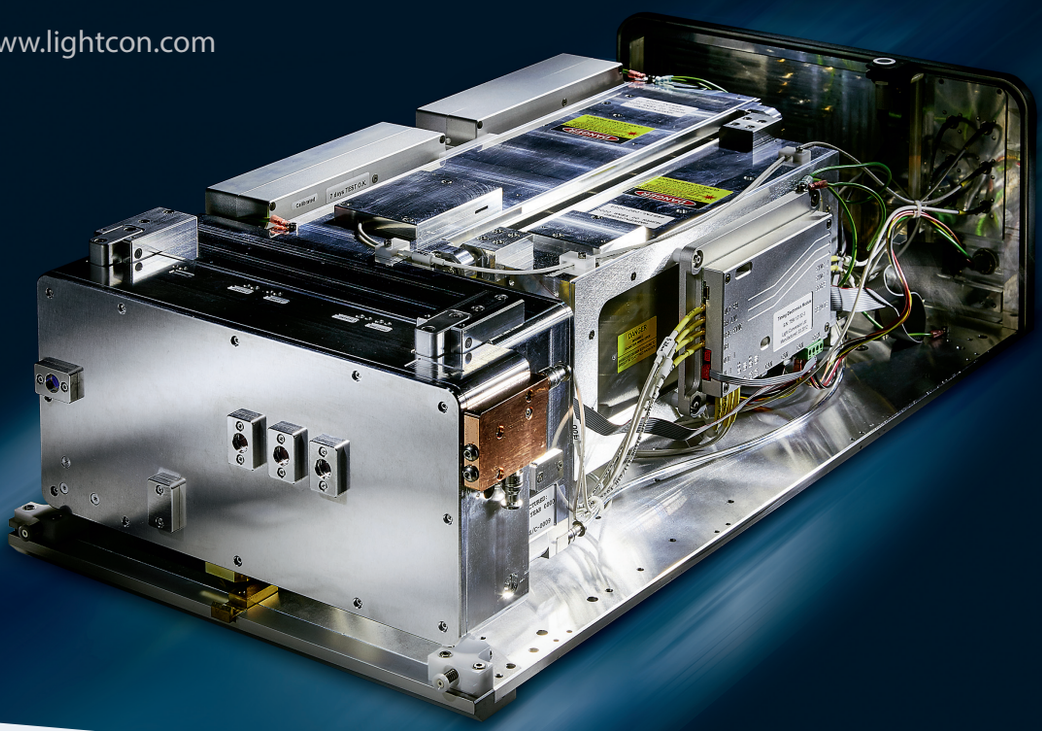

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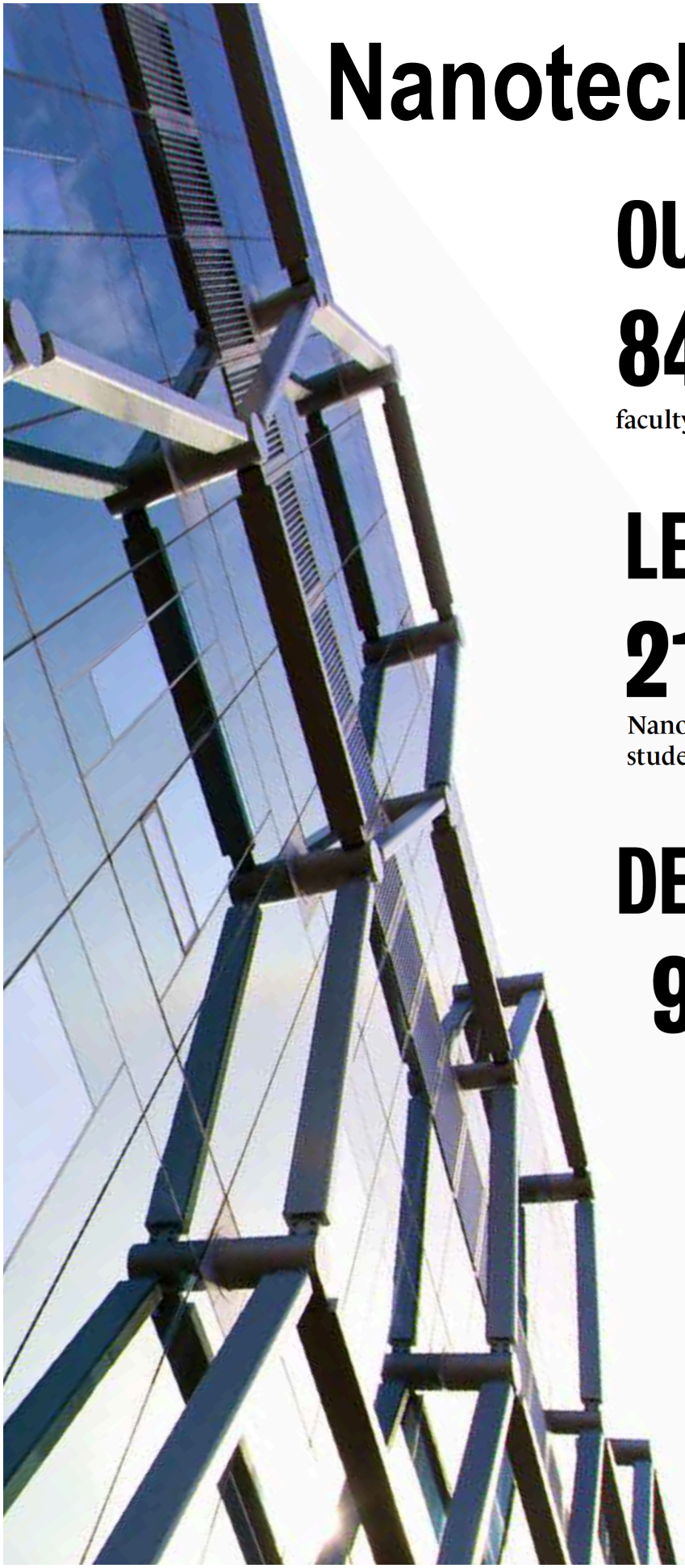


OUR PEOPLE

84 faculty members

20 research chairs

LECTURES

21 Nano graduate student seminars

6 distinguished lectures

18 seminars

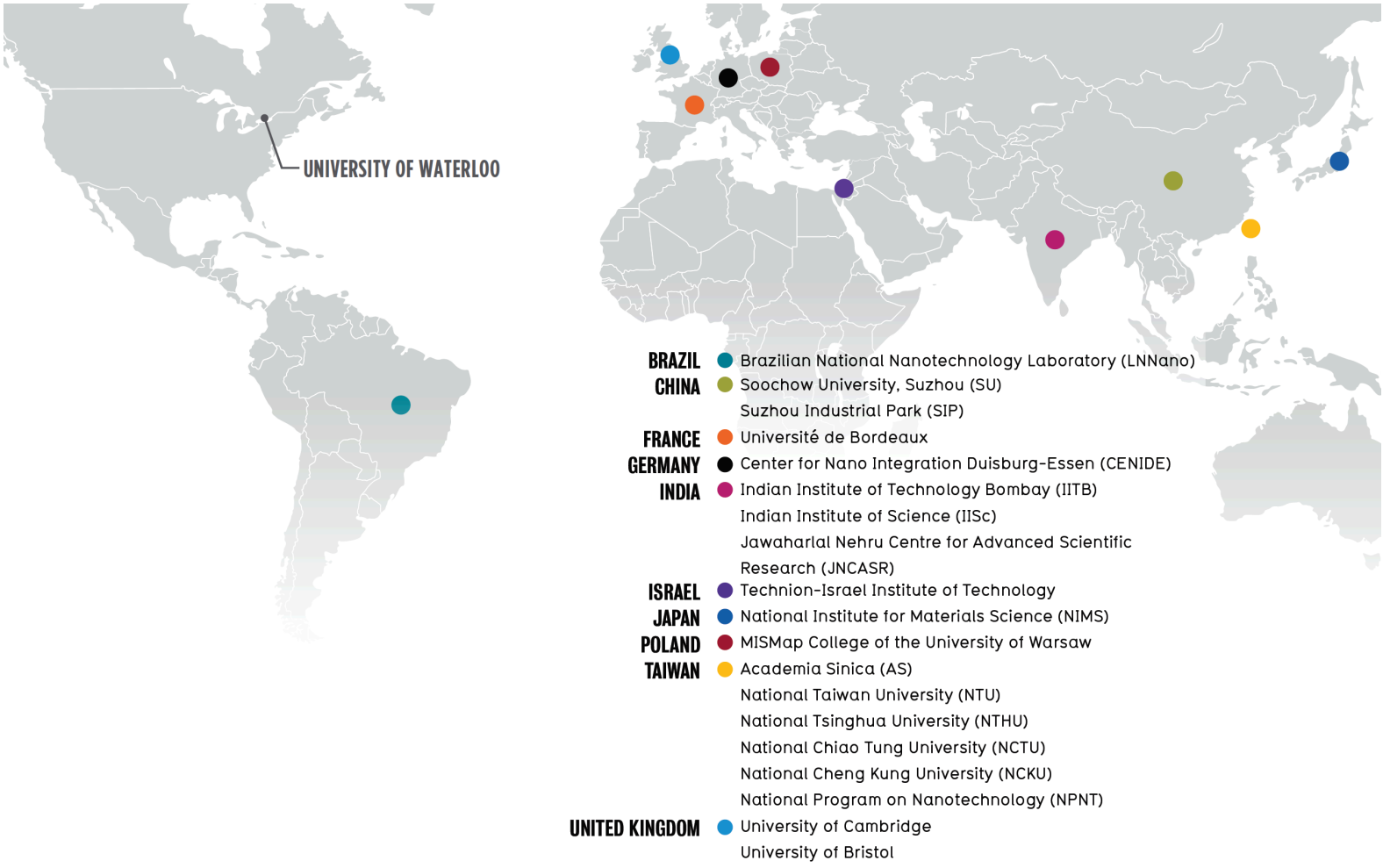
DEPARTMENTS

9

Biology
Chemistry
Chemical Engineering
Electrical & Computer Engineering
Mathematics
Mechnical & Mechatronics Engineering
Systems Design Engineering
Pharmacy
Physics

Cover: Model of graphene, the discovery of graphene was awarded the 2010 Nobel Prize in Physics.

Inside: The exterior of the Quantum Nano Centre is modeled after the hexagonal structure of graphene.



INTERNATIONAL

It's WIN vision to be a GLOBAL centre of excellence in nanotechnology. To that end, internationalization is a central and ongoing activity every year. In 2016, WIN resigned agreements with the top institutes in Japan and Taiwan and participated in workshops with the University of Bristol, and University of Cambridge in the United Kingdom and the Center for Nano Integration Dulburg-Essen (CENIDE) in Germany.

Symposium on Chemical Physics
at the University of Waterloo
November 3-5, 2017

REGISTRATION begins at 6:30 p.m. EIT Foyer

SESSION I: Friday, November 3, 2017 — P.M. EIT-1015
Chair: **Marcel Nooijen**

7:30 – 8:15 **Dvira Segal**
(University of Toronto)
From quantum dynamics to quantum thermodynamics

8:15 – 8:30 **Ramon Miranda Quintana,** Paul W. Ayers
(McMaster University)
Finite-temperature electrophilicity

8:30 – 8:45 **Sarah Henshaw,** Artur Izmaylov
(University of Toronto)
Topological origins of bound states in the continuum for systems with conical intersections

8:45 – 9:00 Brian S. Rolczynski, Haibin Zheng, Ved P. Singh, Polina Navotnaya, Justin R. Caram, **A. Ruvim Ginzburg**[§], Khuram Ashraf, Alastair T. Gardiner[*], Richard J. Cogdell[*], Gregory S. Engel
(University of Chicago; [*]University of Glasgow; [§]present: University of Toronto)
Correlated Nuclear Motions and Electronic Coherence in the Fenna-Matthews-Olson Complex

The Roger E. Miller Lecture is 60 min. including 10 min for discussion.
The D.J. Le Roy Prize Lecture is 20 min including 5 min for discussion
Contributed talks are 15 min. including 3min. for discussion
Invited talks are 45 min. including 5 min. for discussion

9:00 – 11:59 **WELCOME RECEPTION** – GradHouse (GH). *Check your badge, there should be a drink ticket* for the welcome reception. There is also a map of UW campus on the last page of the program; everything is within walking distance.*

***DRINK TICKETS:** You should find a total of **three drink tickets** in your badge. One drink ticket for the **WELCOME RECEPTION (Friday night – GradHouse)**, one drink ticket for the **REFRESHMENTS AND POSTER SESSION (Saturday evening – EIT Upstairs Foyer)**, and one drink ticket for the **AFTERHOURS (Saturday night – GradHouse).**

SESSION II: Saturday, November 4, 2017 – A.M. EIT-1015
Chair: **Pierre-Nicholas Roy**

9:00 – 9:45 **Etienne Garand**
(University of Wisconsin-Madison)
Spectroscopy and chemistry with cryogenic ion traps

9:45 – 10:00 **Paul Johnson**
(Université Laval)
Model wavefunctions for strongly correlated systems

10:00 – 10:15 **Leo Li,** Nathan Seifert, Fan Xie, Yunjie Xu, Wolfgang Jaeger
(University of Alberta)
Proton donor and acceptor strength of hydrogen peroxide: the complicated spectrum of formic acid – H_2O_2

10:15 – 10:45 **COFFEE BREAK**

Invited talks are 45 min. including 5 min. for discussion
Contributed talks are 15 min. including 3 min. for discussion

SESSION III: Saturday, November 4, 2017 – A.M. EIT-1015
Chair: **Scott Hopkins**

10:45 – 11:45 ***The Roger E. Miller Lecture***: **Philippe Maitre**
(Université Paris-Sud; CLIO)
Differential mobility selection and selective infrared fragmentation of small molecular ions

11:45 – 12:00 **Roman Korol,** Michael Kilgour, Dvira Segal
(University of Toronto)
Probing mechanisms of charge transport in DNA with the Landauer-Buttiker formalism

12:00 – 12:15 **Peter Bernath**
(Old Dominion University)
Molecular Astronomy: cool stars and exoplanets

12:15 – 1:30 **LUNCH** – EIT Foyer

SESSION IV: Saturday, November 4, 2017 – P.M. EIT-1015
Chair: **Germán Sciaini**

1:30 – 2:15 So Hirata
(University of Illinois at Urbana-Champaign)
Many-body Green's function theory

2:15 – 2:30 **Karen Morenz,** Minhal Hasham, Mark W.B. Wilson
(University of Toronto)
Chasing bright singlet fission: Monte Carlo simulations and preliminary fluorescence results

2:30 – 2:50 ***The 2015 'D.J. Le Roy Prize' Lecture***: **Steven Gravelsins,** Minhal Hasham, Yi Lin, Kevin Yu, Monique Tie, Cynthia Goh, Al-Amin Dhirani
(University of Toronto)
Self-Assembly of Gold Nanoparticles and Alkanethiols:From Monolayers to Porous Networks

2:50 – 3:05 Isabelle Braud, **Jonathan Vermette,** Pierre-Alexandre Turgeon, Patrick Ayotte, Gil Alexandrowicz*
(Université de Sherbrooke; *Technion, Israel Institute of Tehnology)
Magnetic separation of water spin isomers in a molecular beam

3:05 – 3:20 **Giacinto Scoles**
(Princeton; Elettra)
3D cell cultures combined with single cell metabolism determination and stem cell techniques are poised to solve the nasty problem of rare neuro-degenerative disease diagnostics and cure

The Roger E. Miller Lecture is 60 min. including 10 min for discussion.
The D.J. Le Roy Prize Lecture is 20 min including 5 min for discussion
Contributed talks are 15 min. including 3min. for discussion
Invited talks are 45 min. including 5 min. for discussion

3:25 – 6:00 **REFRESHMENTS AND POSTER SESSION*** EIT Upstairs Foyer

***DRINK TICKETS:** You should find a total of **three drink tickets** in your badge. One drink ticket for the **WELCOME RECEPTION (Friday night – GradHouse)**, one drink ticket for the **REFRESHMENTS AND POSTER SESSION (Saturday evening – EIT Upstairs Foyer)**, and one drink ticket for the **AFTERHOURS (Saturday night – GradHouse).**

SESSION V: Saturday, November 4, 2017 from 3:25 P.M. EIT Upstairs Foyer
POSTER SESSION
Chair: **Marcel Nooijen**

6:00 P.M. **POSTER SESSION ENDS**
Depart for Large Conference Room, ***Federation Hall*** **(FED)**; *check your maps!*

6:30 P.M. **CASH BAR:** Large Conference Room, ***Federation Hall*** **(FED)**

7:00 P.M. **DINNER:** Large Conference Room, ***Federation Hall*** **(FED)**

9:00 P.M. **AFTERHOURS*:** Our band plays at ***GradHouse (GH)!*** *... Informal Discussion.*

***DRINK TICKETS:** You should find a total of **three drink tickets** in your badge. One drink ticket for the **WELCOME RECEPTION (Friday night – GradHouse)**, one drink ticket for the **REFRESHMENTS AND POSTER SESSION (Saturday evening – EIT Upstairs Foyer)**, and one drink ticket for the **AFTERHOURS (Saturday night – GradHouse).**

SESSION VI: Sunday, November 5, 2017– A.M. EIT 1015

Chair: **Pierre-Nicholas Roy**

9:15– 10:00 **Irina Paci**
(University of Victoria)
Dielectric and optical materials with metal nanoparticle inclusions: A theoretical approach

10:00 – 10:15 Wenhao Sun, Rebecca L. Davis, Sven Thorwirth[*], Michael Harding[§], **Jennifer van Wijngaarden**
(University of Manitoba; [*]University of Cologne; [§]Karlsruhe Institute of Technology)
Rotational Spectra and Structure of HCCNCS produced via dc discharge

10:15 – 10:30 **Thomas Halverson,** Pierre-Nicholas Roy
(University of Waterloo)
Entanglement of Rotor Chains

10:30 – 11:00 **COFFEE BREAK**

SESSION VII: Sunday, November 5, 2017– A.M. EIT 1015
Chair: **Germán Sciaini**

11:00 – 11:45 Bradley Siwick
(McGill University)
Ultrafast inelastic electron scattering: Mapping q-dependent electron-phonon coupling and nonequilibrium phonon dynamics in 2D materials

11:45 – 12:00 **Egor Ospadov,** Ilya G. Ryabinkin, Viktor N. Staroverov
(University of Western Ontario)
How to construct exact exchange-correlation potentials for two-electron systems

12:00 – 12:15 Matthias Heger, **Fan Xie,** Zhihao Chen, Joseph Cheramy, Wolfgang Jaeger, Yunjie Xu
(University of Alberta)
Development of hybrid laser-mass spectrometers

12:15 – 1:30 Light **LUNCH & COFFEE** – EIT Foyer

Invited talks are 45 min. including 5 min. for discussion
Contributed talks are 15 min. including 3min. for discussion

IR USERS MEETING: Sunday, November 5, 2017– P.M. EIT 1015
Chair: **Scott Hopkins**

In addition to the regular program, the 2017 Symposium on Chemical Physics will also include an IR Users Meeting on the afternoon of Sunday, November 5th. This meeting will focus on future directions of infrared-based technologies and research in Canada. Attendees will discuss upgrades to the mid- and far-IR beamlines at the Canadian Light Source and the IR free electron laser facility proposed for construction in Waterloo, Ontario. The discussion will be centered around three short presentations of approximately 15 minutes each.

13:30 – 14:00 **Scott Rosendahl**
(Canadian Light Source)
The CLS mid-IR beamline: Capabilities and Proposed Upgrades

14:00 – 14:30 **Brant Billinghurst**
(Canadian Light Source)
Capabilities of and Proposed Upgrades to the CLS far-IR beamline

14:30 – 15:00 **Scott Hopkins**
(University of Waterloo)
A New Canadian IR-FEL Facility

15:00 – 16:00 Additional Discussion

POSTER SESSION: Saturday, November 4, 2017 EIT Upstairs Foyer
Chair: **Marcel Nooijen**

To give people presenting papers in this session an opportunity to both present their work and visit other posters, this session is divided into two time slots:

3:30 – 4:45 Those whose papers were given (a) labels (1a, 2a, 3a, etc.) should attend their posters.
4:45 – 6:00 Those whose papers were given (b) labels (1b, 2b, 3b, etc.) should attend their posters.

1(a) **Allan Adam,** C. Linton, D.W. Tokaryk, H. Zarringhalam
(University of New Brunswick)
High Resolution Spectroscopy of Ruthenium Monofluoride and Ruthenium Monochloride

1(b) **Nigel Andersen**
(University of Waterloo)
An Investigation of Tropylium Ion Complexes in the Gas Phase

2(a) J. Larry Campbell, Yves Le Blanc, Chang Liu, Amol Kafle, Kevin He, Alexandre Wang, **Zack Bowman,** W. Scott Hopkins
(University of Waterloo)
Using differential mobility spectrometry to separate chiral compounds: Amphetamines

2(b) **Patrick Carr,** Stephen Walker, Mike Lecours, Joshua Featherstone, Gau-Lei Hou[*], Xue-Bin Wang[*], Jonas Warneke[*§], Terrance B. McMahon, and W. Scott Hopkins
(University of Waterloo; [*]Pacific Northwest National Laboratory; [§]Universität Bremen)
Gas Phase Studies of $B_{12}X_{122}$- (X=H, F) with All-cis 1,2,3,4,5,6 Hexafluorocyclohexane

3(a) **Isaac De Vlugt,** Dmitri Iouchtchenko, Thomas Halverson and Pierre-Nicholas Roy
(University of Waterloo)
Computing Bound States of Rotor Chains and Arrays Using Direct Operation

3(b) **Randy Dumont**
(McMaster University)
Molecular Electronic Devices - from diodes to refrigerators

4(a) **Amer El-Samman,** Egor Ospadov, Viktor Staroverov
(University of Western Ontario)
Extended Koopmans theorem without numerical difficulties

4(b) **Joshua Featherstone,** Terrance B. McMahon
(University of Waterloo)
An investigation of sodium cyclopentadiene complexes in the gas phase

5(a) **Stijn Fias**
(McMaster University)
Extension of the source-sink potential approach to Hartree Fock and Density Functional Theory: a new tool to visualize the ballistic current

5(b) Yanyang Chen, Graham J. Bodwell, and **Travis D. Fridgen**
(Memorial University)
Structures of Gas-Phase Metal Cation/Aromatic Half-Belt Complexes: Ascertaining Whether Metal Cations Hold or Wear Their Teropyreneophane Belts

6(a) **Weiqiang Fu,** J. Larry Campbell, and W. Scott Hopkins
(University of Waterloo)
The Structures and Properties of the Proton-bound dimer of Phenylalanine with Serine

6(b) **Jiao Gao,** Wolfgang Jaeger
(University of Alberta)
Tautomerism in acetylacetone - water: a spectroscopic and ab initio study

7(a) **Chloe Graham**
(University of Western Ontario)
Investigations into the Dynamics of Calcium Bicarbonate Complexes in Water Clusters

7(b) **Philippe Green,** Philip Sohn, Ruvim Ginzburg, Christian J. Imperiale, Mark W.B. Wilson
(University of Toronto)
Improving Monodispersity in PbS Nanocrystal synthesis via Multi-Component Sulfur Precursors

8(a) **Minhal Hasham,** Karen Morenz, Mark W.B. Wilson
(University of Toronto)
Two-colour fluorescence intermittency spectroscopy

8(b) **Bradley Howie,** Christian Ieritano, W. Scott Hopkins
(University of Waterloo)
Isolation of Isomeric Drug Metabolites by Differential Mobility Spectrometry: A Proof of Concept Study using Caffeine or something like that

9(a) **Christian Ieritano,** Scott Hopkins
(University of Waterloo)
Insights into the Properties of an Anticancer Peptide using Differential Mobility Spectrometry

9(b) **Christian J. Imperiale,** Minhal Hasham, Philippe Green, [*]Thomas J. Carey, Andrew J. Tilley, Dwight S. Seferos, [*]Niels H. Damrauer, Mark W.B. Wilson
(University of Toronto; [*]University of Colorado)
Electronically Decoupled Molecular Dimers for Excitonic Upconversion

10(a) **Dmitri Iouchtchenko,** Martin Ganahl, Isaac De Vlugt, Tom Halverson, Pierre-Nicholas Roy
(University of Waterloo)
Density matrix renormalization group for the ground state of linear chains of linear rigid rotors with dipolar interactions using angular momentum ladder operator

10(b) **Loic Joubert-Doriol,** Artur F. Izmaylov
(University of Toronto)
Exact matrix element nonadiabatic dynamics in the moving crude adiabatic representation

11(a) Nidhi Sinha, Paresh Modak, Suvam Singh, Himani Tomer, Pankaj Verma, **Jaspreet Kaur,** Bobby Antony
(University of Western Ontario)
Electron interaction cross sections for complex biomolecules

11(b) **Victor Kwan,** Stella Constas
(University of Western Ontario)
Computational study of generation of star-shaped nanoparticles to their assembly

12(a) **Arthur Lee,** Steve Walker, Ahdia Anwar, Sarah Ajami, Jarrod Psutka, Chang Liu, Gilles Goetz, John Janiszewski, J. Larry Campbell, W. Scott Hopkins
(University of Waterloo)
Effect of Intramolecular Hydrogen Bonds on Chemical Structure

12(b) **Ronald Lees,** Li-Hong Xu, B.E. Billinghurst[*]
(University of New Brunswick; [*]Canadian Light Source)
Rockin' at the Light Source

13(a) **Su Ji Lim**, Gau-Lei Hou[*], Xue-Bin Wang[*], Jonas Warneke[*§], and W. Scott Hopkins
(University of Waterloo; [*]Pacific Northwest National Laboratory; [§]Universität Bremen)
Photoelectron spectroscopy of $B_{12}X_{12}$, X=H, F, Cl, Br, I

13(b) A.J. Barclay*, A. Mohandesi*, K.H. Michaelian[*], A.R.W. McKellar[§], **Nasser Moazzen-Ahmadi**
(University of Calgary; [*]Natural Resources Canada; [§]National Research Council)
Infrared observation of $OC\text{-}C_2H_2$, $OC\text{-}(C_2H_2)_2$ and their isotopologues

14(a) **Ryan Moreira,** Stephen Walker, Nour Mashmoushi, Scott D. Taylor, W. Scott Hopkins
(University of Waterloo)
Using Differential Mobility Spectrometry to Design Daptomycin Analogs

14(b) **Anand H.G. Patel,** Dr. Ahmed A.K. Mohammed, Dr. Peter A. Limacher[*], Dr. Paul W. Ayers
(McMaster University; [*]Karlsruhe Institute of Technology)
Robust Nonlinear Optical Property Prediction Using a Rational Function Based Finite Field Method

15(a) **Jarrod Psutka,** Pedro A. Segura[*], Annick Dion-Fortier[*], Larry Campbell[§], Scott Hopkins, Thorsten Dieckmann
(University of Waterloo; [*]Université de Sherbrooke; [§]SCIEX)
Separation and Classification of Transformation Products of Trimethoprim Using Differential Mobility Spectrometry

15(b) **Nicolas Rivas,** Tyler Lott, Peter Francis Mathew Elango, Meixin Cheng, Eric Haugen, Ariel Petruk, Kostyantyn Pichugin, German Sciaini
(University of Waterloo)
Sample Preparation and Delivery Methods for Ultrafast Nonlinear Optical Studies at UeIL

16(a) **Stephanie Ryall,** Jarrod Psutka, Larry Campbell, W. Scott Hopkins
(University of Waterloo)
Separation of Tautomers of Protonated Methylated Nucleobases

16(b) **Tapas Sahoo,** Dmitri Iouchtchenko, Pierre-Nicholas Roy
(University of Waterloo)
Computation of ground state entanglement entropy for angular motion of many rotors using path integral imaginary time dynamics

17(a) **Matthew Schmidt,** Pierre-Nicholas Roy
(University of Waterloo)
Quantum Molecular Dynamics Simulations of the Water Monomer and Dimer in the Ground State

17(b) **Philip Sohn,** Philippe Green, Mark W.B. Wilson
(University of Toronto)
The Mechanism of PbS Colloidal Nanocrystal Synthesis Via Thioureas and Analogous Precursors

18(a) **Wenhao Sun,** Jennifer van Wijngaarden
(University of Manitoba)
Microwave spectral detection of long carbon chain species newly formed in discharge jet: HCCCCNCS & NCCCNCS

18(b) Nicholas S. Caron, Colan Linton, **Dennis W. Tokaryk,** Allan G. Adam
(University of New Brunswick)
Spectroscopy and direct potential fitting of the $X_1\Sigma^+$, $A_1\Pi$ and $B_1\Sigma^+$ electronic states of MgS

19(a) **Li-Hong Xu,** E.A. Alekseev[*], S.P. Belov[§], G.Yu. Golubiatnikov[§], J.T. Hougen[¶]
(University of New Brunswick, [*]Kharkiv, [§]NNOV, [¶]NIST)
Nuclear spin-rotation and spin-torsion interactions in Methanol

19(b) Fan Xie, Jason T. A. Gall, Leo Li, Javix Thomas, Wenyuan Huang, Zhibo Wang, Wolfgang Jäger, **Yunjie Xu**
(University of Alberta)
Asymmetric water tunneling paths in (chiral) molecule-water complexes

20(a) **Spencer Yim**
(University of Waterloo)
Entanglement Entropy of Quantum Fluids

20(b) **Ce Zhou,** Amy Yang, Mike Lecours, Stephen Walker, Rick A. Marta, Eric Fillion, Terry McMahon, Larry Campbell, W. Scott Hopkins
(University of Waterloo)
Structures and Properties of Serine Clusters

21(a) **Ariel Petruk,** Aly Hassan, Nicolás Rivas, Kostyantyn Pichugin, Germán Sciaini
(University of Waterloo)
Development of time-resolved electron microscope and its accessories at UeIL

21(b) **Laura Durán Caballero,** Ricardo Pérez de Tudela[*], Dominik Marx
(Ruhr-Universität Bochum, [*]University of Waterloo)
Water Microsolvation of Non-zwitterionic versus Zwitterionic Glycine

22(a) **Ignacio Loaiza,** Artur Izmaylov
(University of Toronto)
Comparative assessment of surface hopping and Ehrenfest methods for molecular dynamics on metallic surfaces

22(b) **Isabelle Braud,** Jonathan Vermette, Pierre-Alexandre Turgeon, Patrick Ayotte, Gil Alexandrowicz[*]
(Université de Sherbrooke; [*]Technion, Israel Institute of Tehnology)
Magnetic separation of water spin isomers in a molecular beam

23(a) **Ruodi Cheng,** Victoria Rose, Travis D. Fridgen
(Memorial University)
The IRMPD and computational study of 1-methylcytosine and 9-ethylguanine base pair with alkali metal cation and proton

23(b) **Qiuying Zhang,** Stephen Walker, J.Larry. Campbell, Steven Innocente, W. Scott Hopkins
(University of Waterloo)
Characterizing humulone content in beer

24(a) **Jianying Sheng,** Michel Gingras, and Pierre-Nicholas Roy
(University of Waterloo)
Confined Quantum Molecular Degrees of Freedom

Notes

SUPPLEMENTARY INFORMATION

- **Poster Preservation**
  In past years, posters left up after the poster session have sometimes been vandalized during the night. If you wish to avoid this possibility, take down your poster after the session Saturday afternoon, before leaving for the Conference Dinner.

- **Recycling**
  Before leaving on Sunday, please drop you plastic name-tag holder into the cardboard box by the entrance to the Registration area. This will allow recycling and reduced our costs for next year.

- **Phone Numbers**:
  Airways Transit: 519-886-2121 https://secure.airwaystransit.com
  Waterloo Taxi: 519-886-1200
  United Taxi: 519-888-0400
  City Cab: 519-747-7777

Please note that Waterloo Taxi offers flat rates to airport locations, which are usually cheaper than Airways Transit!

PARKING LOTS FOR VISITORS AND RATES

The following parking lots are available for use by visitors to campus;

- Parking Lot C - $5.00
- Parking Lot N - $5.00
- Parking Lot W - $5.00
- Parking Lot M - $6.00
- Parking Lot X - $5.00 (Free on Weekends beginning on Fridays at 4:30p.m)

Parking Lot H - $2.00 hourly Max $10 (**during non co-op days**)
After 3:45 p.m H Lot is a flat rate of $5.00 as well as on weekends.

Parking Lot D - $2.00 hourly Max $15
After 3:45 p.m D lot is flat rate of $5.00 as well as on weekends.

Reservations for both D lot and H lot can be sent to uparking@uwaterloo.ca and more information for both D and H lot can be found here

Entry machines at D and H lot will only take MasterCard or Visa. It will not accept Amex, Tim Hortons Visa, MasterCard Debit or Visa Debit. There are signs on the machine at both the entrance and exit to indicate same. There are help buttons on all machines which will ring into the office.

Lots B, R, A, are available for entry by coin evenings and weekends after 3:45 pm at a cost of $5.00

***Parking lots T and L are not available for visitors at any time.

UNIVERSITY OF WATERLOO MAP

Arrows indicate the most important locations for our symposium
EIT = Centre for Environmental and Information Technology
FED = Federation Hall. Here we have our dinner on Saturday starting at 7 pm.
GH = GradHouse. Here we have our welcome reception (Friday) and afterhours (Saturday)