Sagamore 2018 Programme

Sunday - 8 July

2:00 - 5:00 pm	*Registration*		
5:00 - 5:20 pm	*Walk to Sackville Landing on the waterfront, behind the Maritime Museum, at 1655 Lower Water Street, to board the Tall Ship Silva for a chartered cruise of historic Halifax Harbour.*		
5:30 - 7:30 pm	**WELCOME RECEPTION** *While enjoying scenic Halifax from the deck of a majestic ship in the harbour, greet your colleagues while enjoying local wines and hors d'oeuvres.*		

Monday - 9 July

9:00 - 9:10 am	*Opening remarks by Conference Chair and Co-Chair*	**Chérif F. Matta** **Paul W. Ayers**	
Start: 9:10 am End: 12:00 pm	**SESSION 1:** ***Ultrafast science and molecular imaging***	**Chair:** **Pierre-Nicolas Roy**	
9:10 - 9:20 am	*Introductory remarks by Session Chair*	**Pierre-Nicolas Roy**	
9:20 - 10:00 am	Plenary: *Mapping atomic motions with ultrabright electrons: Fundamental space-time limits to imaging chemistry*	**R. J. Dwayne Miller**	30
10:00 - 10:20 am	*Many-electron effects in calculated laser-induced electron diffraction spectra of laser-driven molecules*	**T. Tung Nguyen-Dang**	31

Monday - 9 July

10:20 - 10:40 am	**COFFEE BREAK**		
10:40 - 11:20 am	Plenary: *Circular polarization in attosecond phenomena and applications*	**André D. Bandrauk**	32
11:20 am - 12:00 pm	Plenary: *Molecular movies from ultrafast time-resolved gas phase x-ray scattering*	**Peter M. Weber**	33
12:00 - 1:40 pm	**LUNCH**		
1:40 - 2:00 pm	*Exploring the quantum / electron crystallography nexus*	**Philip Nakashima**	35
	END OF SESSION 1		
Start: 2:00 pm End: 3:50 pm	**SESSION 2:** ***Non-conventional materials: Confined, frustrated, nanocrystaline, plasmonic, and magnetic materials***	**Chair:** **Philip Nakashima**	
2:00 - 2:10 pm	*Introductory remarks by Session Chair*	**Philip Nakashima**	
2:10 - 2:30 pm	*Quantum effects and properties of nanoconfined molecular rotors?*	**Pierre-Nicholas Roy**	38
2:30 - 2:50 pm	*Nano cool, micro cooler! What do we want in our plasmonic materials, bandgap or no bandgap?*	**Vaibhav Thakore**	39

Monday - 9 July

2:50 - 3:10 pm	*Joint refinements on $YTiO_3$: State of the art and first steps to the wave functions refinement*	**Nicolas Claiser**	40
3:10 - 3:30 pm	*Donor-acceptor stabilization of, and bonding in, lowoxidation state main group element hydrides*	**Alex Brown**	42
3:30 - 3:50 pm	*Novel nanocrystalline material and their application*	**Khashayar Ghandi**	43
	END OF SESSION 2		
3:50 - 4:10 pm	**COFFEE BREAK**		
Start: 4:10 pm End: 5:40 pm	**SESSION 3:** ***Matter under extreme conditions and induced phase transitions***	**Chair:** **Piero Macchi**	
4:10 - 4:20 pm	*Introductory remarks by Session Chair*	**Piero Macchi**	
4:20 - 5:00 pm	Plenary: *On the control parameters of pressure-induced bond activation/compression*	**Wolfgang Scherer**	44
5:00 - 5:20 pm	*Atomic and molecular properties of diatomic molecules in external electric fields*	**Shahin Sowlati-Hashjin**	46
5:20 - 5:40 pm	*Bonding formation along the pressure-induced B3-B1 phase transition in InP*	**Jose Manuel Recio**	48
	END OF SESSION 3		

Monday - 9 July

5:40 - 5:50 pm	Short out of sequence talk: *Pentacoordinated silicon compounds as a model system to study SN_2 reactions*	**Malte Fugel**	50
6:00 - 9:00 pm	**POSTER SESSION & COCKTAIL** (Including Poster Prizes competition and vote)		

Tuesday - 10 July

Start: 9:00 am End: 10:40 am	**SPECIAL AWARDS SESSION**	**Chair:** **Carlo Gatti**	
9:00 - 9:05 am	*Remarks by the Session Chair*	**Carlo Gatti**	
9:05 - 9:10 am	*Introductory remarks by the Chair of the (Early Career) Miguel A. Blanco Prize Selection Committee*	**Carlo Gatti**	
9:10 - 9:50 am	The Miguel A. Blanco Prize Lecture: *The pair density as a source of chemical information*	**Eduard Matito**	52
9:50 - 9:55 am	SHORT 5 MINUTES BREAK		
9:55 - 10:00 am	*Introductory remarks by a member of the (Advanced Career) Richard F. W. Bader Prize Selection Committee*	**T. Tung Nguyen-Dang**	
10:00 - 10:40 am	The Richard F. W. Bader Prize Lecture: *Topologically partitioned electron correlation energy*	**Paul L. A. Popelier**	53

Tuesday - 10 July

	END OF SPECIAL AWARD SESSION		
10:40 am - 11:00 am	**COFFEE BREAK**		
Start: 11:00 am End: 4:40 pm	**SESSION 4:** ***Advances in the theoretical and experimental studies of the electron density***	**Chair:** **Wolfgang Scherer**	
11:00 - 11:10 am	*Remarks by the Session Chair*	**Wolfgang Scherer**	
11:10 - 11:30 am	*Electron counting in position space: From quantum fragments to Lewis structures to multicenter bond*	**Ángel Martín Pendás**	56
11: 30 - 11:50 am	*Density meets orbitals*	**Lukas Bucinsky**	57
11:50 am - 12:00 pm	Short talk: *X-ray charge density study of chemical bonding in ZnSb*	**Hidetaka Kasai**	58
12:00 – 1:40 pm	**LUNCH**		
	SESSION 4 (Cont'd)		
1:40 - 2:20 pm	Plenary: *Electron density and real structure of materials*	**Yuri Grin**	60
2:20 - 2:40 pm	*Electron density from strong-correlation wave functions*	**Markus Reiher**	62
2:40 -3:00 pm	*How do density functional approximations affect our results?*	**Julia Contreras-García**	63

Tuesday - 10 July

3:00 - 3:20 pm	*The topological structure of complex molecules: Challenges and near future directions*	**Hugo J. Bohórquez**	65
3:20 - 3:40 pm	*Comprehensive electron density analysis of 1 to 3D systems fully integrated in the ab initio CRYSTAL code*	**Silvia Casassa**	67
3:40 - 4:00 pm	**COFFEE BREAK**		
4:00 - 4:20 pm	*Next generation QTAIM*	**Samantha Jenkins**	69
4:20 - 4:40 pm	*The electron density at the complete basis set limit*	**SeyedAbdolreza Sadjadi**	71
	END OF SESSION 4		
Start: 4:40 pm End: 5:50 pm	**SESSION 5:** ***Electron density in catalysis & enzymology***	**Chair:** **Julia Contreras-García**	
4:40 - 4:50 pm	*Remarks by the Session Chair*	**Julia Contreras-García**	
4:50 - 5:10 pm	*Enzymatic reaction modelling as a stretch-test of machine learning based on small-molecule electron density topological training data*	**Preston J. MacDougall**	73
5:10 - 5:30 pm	*The catalytic role of hydrogen bond interactions*	**Aurora Costales**	75
5:30 - 5:50 pm	*Sila-Ibuprofen and interaction densities in crystal vs. enzyme environments*	**Simon Grabowsky**	76

Tuesday - 10 July

	END OF SESSION 5		
6:00 - 9:00 pm	*Open meeting of the IUCr's Commission on Quantum Crystallography (CQCr)*	*IUCr-CQCr Members @ Sagamore 2018:* **E. Espinosa, J. Kozisek, C. F. Matta, E. Nishibori, W. Scherer** *IUCr-CQCr Consultants @ Sagamore 2018:* **P. Macchi, C. Gatti, J. Contreras-Garcia, Y. Sakurai**	

Wednesday - 11 July

Start: 9:00 am End: 2:20 pm	**SESSION 6:** ***Synergy of experiment and theory in crystallography***	**Chair:** **Dylan Jayatilaka**	
9:00 - 9:10 am	*Introductory remarks by Session Chair*	**Dylan Jayatilaka**	
9:10 - 9:50 am	Plenary: *In good experiments we can trust!*	**Dietmar Stalke**	78
9:50 - 10:10 am	*Libraries of extremely localized molecular orbitals and their coupling to Hirshfeld atom refinement*	**Alessandro Genoni**	80
10:10 - 10:30 am	*Comparison of experimental and theoretical results of electronic structure of 3-(2'-tetrahydropyranyloxy)-4- methylthiazole-2(3H)-thione*	**Jozef Kožíšek**	82
10:30 am - 11:00 am	**COFFEE BREAK**		

Wednesday - 11 July

11:00 - 11:20 am	*Quantum crystallography (QCr): Early views & recent ideas*	**Lou Massa**	84
11:20 - 11:40 am	*Experimental and theoretical structure factors of simple metal oxides*	**Eiji Nishibori**	85
11:40 am - 12:00 pm	*A method to estimate statistical errors of properties derived from charge density modeling*	**Benoît Guillot**	88
12:00 - 1:40 pm	**LUNCH**		
	SESSION 6 (Cont'd):		
1:40 - 2:00 pm	*Methods development for charge density studies of actinide compounds: from data reduction to model building*	**Christopher G. Gianopoulos**	89
2:00 - 2:20 pm	*Removing residual bond density in organic molecules: A technical note*	**Alexander Y. Nazarenko**	90
	END OF SESSION 6		
Start: 2:20 pm End: 5:30 pm	**<u>SESSION 7:</u>** ***Modern approaches to chemical bonding & aromaticity***	**<u>Chair:</u>** **Ángel Martín Pendás**	
2:20 - 2:30 pm	*Introductory remarks by Session Chair*	**Ángel Martín Pendás**	
2:30 - 2:50 pm	*Evaluation of spatial domains*	**Miroslav Kohout**	92

Wednesday - 11 July

2:50 - 3:10 pm	*Characterizing the halogen and chalcogen bonds in crystals: PAEM vs ESP*	**Ekaterina Bartashevich**	93
3:10 - 3:30 pm	*Charge density analysis of triphosphazenes: Aromaticity and the NCl unit*	**Fernando Cortés-Guzmán**	96
3:30 - 4:00 pm	**COFFEE BREAK**		
4:00 - 4:20 pm	*How real-space bonding indicators can help in description of the nature of donor acceptor bonds*	**Lilianna Chęcińska**	97
4:20 - 4:40 pm	*Stacking of planar polyenic rings: From dispersion interactions to multicentric two-electron covalent bonding*	**Krešimir Molčanov**	98
4:40 - 5:00 pm	*What does electron density analysis tell us about bonding in transition metal-doped boron and carbon clusters?*	**N. Sukumar** *(via video conferencing)*	100
	END OF SESSION 7		
5:00 – 5:45 pm	**Sagamore 2018 Group Photo**		
5:45 - 6:00 pm	**TRANSIT TIME**		
6:00 - 9:00 pm	**Sagamore 2018 Banquet** (Including celebration of the Sagamore 2018 international awards laureates & announcing poster prizes winners)		

Thursday - 12 July

Start: 9:00 am End: 10:10 am	**SESSION 8:** ***Advanced characterization, detection, and inelastic scattering***	**Chair:** **Vaibhav Thakore**	
9:00 - 9:10 am	*Introductory remarks by Session Chair*	**Vaibhav Thakore**	
9:10 - 9:30 am	*Spin-resolved momentum densities: What we can learn from magnetic Compton scattering*	**Jon Duffy**	103
9:30 - 9:50 am	*Advanced spectroscopic characterization of lithium-ion battery materials using x-ray Compton scattering*	**Hasnain Hafiz**	105
9:50 - 10:10 am	*Nonlinear optical microscopy for discriminating tissues based on ultrastructure*	**Danielle Tokarz**	106
	END OF SESSION 8		
Start: 10:10 am End: 12:00 pm	**SESSION 9:** ***Advanced material design and structure-to-property relationships***	**Chair:** **Miroslav Kohout**	
10:10 - 10:20 am	*Introductory remarks by Session Chair*	**Miroslav Kohout**	
10:20 - 10:40 am	*Phonon-mediated high-temperature superconductivity?*	**Roman Krems**	108
10:40 - 11:00 am	**COFFEE BREAK**		
11:00 - 11:20 am	*Design of macrocyclic chelating agents with actinium for development of targeted radiotherapy*	**Amanda Morgenstern**	109

Thursday - 12 July

11:20 am - 11:40 am	*Structure-property relationships in an ambipolar organic semiconductor cum NLO material: New insights from energy frameworks and charge density analysis*	**Parthapratim Munshi**	110
11:40 - 12:00 am	*Revisiting the structure of "*Pbca*"* (±)-*[Co(en)$_3$]I$_3$.H$_2$O - Comparing the results obtained by x-ray and neutron diffraction with those predicted with PLATON and the flack test when using x-ray data alone*	**Ivan Bernal**	112
	END OF SESSION 9		
12:00 - 1:40 pm	**LUNCH**		
Start: 1:40 pm End: 2:50 pm	**SESSION 10:** ***Electron delocalization descriptors in material and catalyst design***	**Chair:** **Enrique Espinosa**	
1:40 - 1:50 am	*Introductory remarks by Session Chair*	**Enrique Espinosa**	
1:50 - 2:30 pm	Long Talk: *The many faces of localization-delocalization matrices*	**Ronald L. Cook**	113
2:30 - 2:50 pm	*Use of differential electron density to elucidate the origins of stereoselectivity in synthetic organic reactions*	**Paul Ha-Yeon Cheong**	115
	END OF SESSION 10		

Thursday - 12 July

2:50 - 3:10 pm	Out of sequence talk: *Half-metallicity of graphite-like and amorphous carbon nanoparticles and their potential applications in spin catalysis: Quantum chemistry predictions*	**Gilles Peslherbe**	117
3:10 - 4:45 pm	**FREE TIME**		
	EXCURSION DINNER		
5:00 - 9:00 pm	Bus charter excursion to scenic Peggy's Cove, to enjoy a walk on the majestic rocks and a light dinner at the on-site restaurant		

Friday - 13 July

9:00 - 10:20 am	**Round Table 1:** ***Quantum Crystallography: Past, Present, and Future***	**Carlo Gatti, Enrique Espinosa, Dylan Jayatilaka, Piero Macchi, Masaki Takata**
10:20 - 10:40 am	**COFFEE BREAK**	
10:40 - 12:00 am	**Round Table 2:** ***Experiment & Theory: Can the Synergy be Furthered?***	**Carlo Gatti, Enrique Espinosa, Dylan Jayatilaka, Piero Macchi, Masaki Takata**
12:00 - 12:10 am	Closing remarks from the Chair and Co-chair of Sagamore 2018	**Chérif F. Matta** **Paul W. Ayers**
12:10 pm	**ADJOURNMENT – FAREWELL**	

POSTER SESSION*
Monday – 9 July (6:00 pm – 9:00 pm)

Posters are listed in alphabetical order by the family name of the presenting author:

Poster number	Title	Presenting Author	
1	*On the thermodynamic stability and the natural selection of canonical nucleosides in the prebiotic evolution of life*	**Lázaro A. Monteserín Castanedo**	120
2	*A "direct" mechanism for the action of the genoprotectors extracted from the Cuban plant* Phyllanthus Orbicularis K	**Lázaro A. Monteserín Castanedo**	122
3	*Interpretation of the Kernel Energy Method (KEM) using the theory of Interacting Quantum Atoms (IQAs)*	**Youji Cheng**	124
4	*IP data correction for accurate charge density study*	**Yuka Deguchi**	125
5	*Theoretical study of electron density and energy transfer in photophysical processes*	**Jesús Hernández- Trujillo**	128
6	*Determination of spin and orbital moments in $Nd_2Ir_2O_7$ using magnetic Compton scattering*	**Daniel O'Neill**	130
7	*Total X-ray wavefunction refinement*	**Rumpa Pal**	131
8	*Experimentally refined density functional theory on strongly correlated materials*	**Ding Peng**	133

* Two Poster Prize winners will be announced at the Conference Banquet. Winner will be selected by a voting process from the posters displayed at the poster session.

POSTER SESSION*
Monday – 9 July (6:00 pm – 9:00 pm)

Posters are listed in alphabetical order by the family name of the presenting author:

9	*The chemistry of transition metal structure*	**Malavikha Rajivmoorthy**	136
10	*Electron density redistribution during a photoinduced geometrical change of copper (I) complexes*	**David Ramírez- Palma**	137
11	*Theoretical study of reactions mediated by ternary Cu(II) complexes*	**Lillian Gisela Ramírez-Palma**	139
12	*Pinpointing origins of selectivity with dimensionally reduced electron density*	**H. Camille Richardson**	141
13	*X-ray charge density study of molybdenum*	**Tomoaki Sasaki**	142
14	*Computational investigation of polyhexamethylene biguanide (PHMB) mechanism of action on the bacterial membrane*	**Shahin Sowlati- Hashjin**	144
15	*Gradient bundle analysis — Full volumetric charge density behavior in a single plot*	**Tim Wilson**	145

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