



10th Congress of the World Association of Theoretical and Computational Chemists

Advances in Electronic Structure Theory; Chemical Reactions and Catalysis; Time Dependent Phenomena; Ab Initio Quantum Chemistry; Spectroscopy; DFT; Advanced Materials; Spin; QM/MM; Energy Conversion and Storage...

WATOC Program for Sunday October 5, 2014

Timing	Sunday 5
14:00-20:00	Registration
16:00-16:40	Opening Ceremony
16:40-17:00	IC000
17:00-17:45	PL1
17:45-20:00	Chilean Dances & Welcome Cocktail

The registration desk will be open from 14:00, it will remain open until 20:00.

Opening Ceremony:

16:00-16:10: Words by Professor Ignacio Sanchez, President of PUC.

16:10-16:20: Words by the Dean of the Faculty of Chemistry at PUC, Prof. Bárbara Loeb.

16:20-16:30: Words from the Organizers, Professor Alejandro Toro-Labbé.

16:30-16:40: Words by the President of WATOC, Prof. Walter Thiel (Germany).

16:40-17:00: Invited Conference **IC000** by Professor Leo Radom (Australia): **The Tenth Congress of WATOC: Reflections on its Origins and Growth.**

17:00-17:45: Plenary Lecture **PL1** by Professor Manuel Yáñez (Spain): **From Old Bonding Patterns to New Enhanced Reactivity Trends.**

17:45-20:00: Break, Chilean Dances and Welcome Cocktail.



10th Congress of the World Association of Theoretical and Computational Chemists

Advances in Electronic Structure Theory; Chemical Reactions and Catalysis;
Time Dependent Phenomena; Ab Initio Quantum Chemistry; Spectroscopy;
DFT; Advanced Materials; Spin; QM/MM; Energy Conversion and Storage...

WATOC Program for Monday 6 to Thursday 9

Timing	Monday 6	Tuesday 7	Wednesday 8	Thursday 9
8:30 -9:15	PL2	PL4	PL6	PL8
9:15-10:00	PL3	PL5	PL7	PL9
10:00-10:30	Coffe Break	Coffe Break	Coffe Break	Coffe Break
10:30-10:55	IC001-005	IC046-050	IC091-095	IC121-125
10:55-11:20	IC006-010	IC051-055	IC096-100	IC126-130
11:20-11:45	IC011-015	IC056-060	IC101-105	IC131-135
11:45-12:10	IC016-020	IC061-065	IC106-110	IC136-140
12:10-12:35	Lunch & Posters Session 1 (PP001-PP190)	Lunch & Posters Session 2 (PP191-PP376)	IC111-115	Lunch & Poster Session 3 (PP377-PP568)
12:35-13:00			IC116-120	
13:00-13:25 13:25-13:50 13:50-14:15				
14:15-14:40	IC021-025	IC066-070	F R E E A F T E R N O N	IC141-145
14:40-15:05	IC026-030	IC071-075		IC146-150
15:05-15:30	IC031-035	IC076-080		IC151-155
15:30-15:55	IC036-040	IC081-085		IC156-160
15:55-16:20	IC041-045	IC086-090		IC161-165
16:20-16:40	Coffe Break	Coffe Break		Coffe Break
16:40-16:55	OP001-005	OP031-035		OP061-065
16:55-17:10	OP006-010	OP036-040		OP066-070
17:10-17:25	OP011-015	OP041-045		OP071-075
17:25-17:40	OP016-020	OP046-050		OP076-080
17:40-17:55	OP021-025	OP051-055		OP081-085
17:55-18:10	OP026-030	OP056-060		OP086-090
18:10-19:30	Poster Session 1 (PP001-PP190)	Poster Session 2 (PP191-PP376)		Poster Session 3 (PP377-PP568)
19:30-22:00				WATOC 2014 Dinner



10th Congress of the World Association of Theoretical and Computational Chemists

Advances in Electronic Structure Theory; Chemical Reactions and Catalysis; Time Dependent Phenomena; Ab Initio Quantum Chemistry; Spectroscopy; DFT; Advanced Materials; Spin; QM/MM; Energy Conversion and Storage...

WATOC Program for Friday October 10, 2014

Timing	Friday 10
8:30-9:15	PL10
9:15-10:00	PL11
10:00-10:30	Coffe Break
10:30-10:55	IC166-170
10:55-11:20	IC171-175
11:20-11:45	IC176-180
11:45-12:10	IC181-185
12:10-12:35	Lunch
12:35-13:00	
13:00-13:25	
13:25-13:50	IC186-190
13:50-14:15	IC191-195
14:15-14:40	IC196-200
14:40-14:55	OP091-095
14:55-15:10	OP096-100
15:10-15:25	OP101-105
15:25-15:40	OP106-110
15:40-16:30	Closing Ceremony

Special Sessions:

In Memoriam of the late Professor Rubén Contreras: Monday 06, 14:45-16:20, Room 4.

Chair: Gustavo E. Scuseria (USA).

Session celebrating 50 years of the Hohenberg-Kohn Theorems: Wednesday 08, 10:30-13:00, Room 1. **Chair: Prof. Paul Geerlings (Belgium).**



10th Congress of the World Association of Theoretical and Computational Chemists

Advances in Electronic Structure Theory; Chemical Reactions and Catalysis; Time Dependent Phenomena; Ab Initio Quantum Chemistry; Spectroscopy; DFT; Advanced Materials; Spin; QM/MM; Energy Conversion and Storage...

WATOC 2014: Plenary Lectures (PL)*

Lecture	Date	Title	Lecturer
PL1	SUNDAY 5 17:00	From Old Bonding Patterns to New Enhanced Reactivity Trends	Manuel Yáñez (Spain)
PL2	MONDAY 6 8:30AM	Concepts for Organizing Chemical Knowledge	Paul W. Ayers (Canada) 2012 Dirac Medal.
PL3	MONDAY 6 9:15AM	Fragmentation: A Route to Accurate Calculation on Large Molecular Systems	Mark Gordon (USA) 2014 Schrödinger Medal,
PL4	TUESDAY 7 8:30AM	(Photo)Electrocatalysis: Theory and Mechanisms of Charge Transfer at Metal Surfaces	Emily Carter (USA)
PL5	TUESDAY 7 9:15AM	Multiscale Modeling of Complex Biological Systems and Processes	Arieh Warshel (USA)
PL6	WEDNESDAY 8 8:30AM	Optical Spectra with Time-Dependent Density Functional Theory	Denis Jacquemin (France) 2014 Dirac Medal
PL7	WEDNESDAY 8 9:15AM	Modeling of Complex Chemical Processes by Dispersion-Corrected DFT	Stefan Grimme (Germany) 2013 Schrödinger Medal
PL8	THURSDAY 9 8:30AM	From One to Many-Electrons Chemical Bonds	Marco A. Chaer Nascimento (Brazil)
PL9	THURSDAY 9 9:15AM	A Variational Approach to Enhanced Sampling and Free Energy Calculations	Michele Parrinello (Switzerland)
PL10	FRIDAY 10 8:30AM	New Tools for Ab Initio Molecular Electronic Structure Calculations of Ground and Excited States	Filipp Furche (USA) 2013 Dirac Medal
PL11	FRIDAY 10 9:15AM	Relativistic Quantum Chemistry: The Broad Picture and Some Recent Results	Pekka Pyykkö (Finland) 2012 Schrödinger Medal

*All Plenary Lectures will be presented in Room 2