



ICCMSE 2016
Metropolitan Hotel, Athens, Greece,
17-20 March 2016

17 March 2016		
SESSION: Computational Chemistry (CC) Symposium		
Honorary Lecture (1) & Organizer Lecture (1)		
CHAIR: Taku Onishi & Tokuei Sako		
(ROOM 1)		
08:50 – 09:00	Opening Ceremony	
09:00 – 10:00	Honorary Lecture Cleanthes A. Nicolaides	Quantum Chemistry on the time axis: Electron correlations and rearrangements on femtosecond and attosecond scales
10:00 – 10:30	Taku Onishi	Computational Chemistry (CC) symposium in ICCMSE 2016
10:30 – 10:50	Coffee Break	

17 March 2016		
SESSION: Computational Modeling of Photonics, Nanophotonics and Metamaterials		
CHAIR: Tatjana Gric		
(ROOM 2)		
09:00 – 09:30	H. Jaffres, T. Fordos, K. Postava, J. Pistora, H.-J. Drouhin	Model and calculations of spin-vecels properties in optical cavities via s-matrix formalism
09:30 – 10:00	H.Fujii, S. Okawa, Y. Yamada, Y. Hoshi, M. Watanabe	Normalization method of highly forward-peaked scattering phase function using the double exponential formula for radiative transfer
10:00 – 10:30	E. Miyakawa, H. Fujii, K. Hattori, Y. Tatekura, K. Kobayash,i M. Watanabe	Numerical study of photon migration in the presence of a void region using the radiative transfer and diffusion equations



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17 March 2016 SESSION: GENERAL SESSION I CHAIR: Andrzej Katunin (ROOM 3)		
09:00 – 09:30	<i>Feng Gong, Hai M. Duong and Dimitrios V. Papavassiliou</i>	Mesoscopic Modeling of Heat Transfer in Carbon Nanotube Multiphase Polymer Composites
09:30 – 10:00	<i>S. Woods and W. Szyszkowski</i>	Integrating Finite Elements with Optimal Control to Simulate Active Vibrations Attenuation
10:00 – 10:30	<i>Andrzej Katunin</i>	Generalized chemical distance distribution in all-sided critical percolation clusters
10:30 – 11:00	<i>N. A. Enaki</i>	Cooperative Entangled Effects Between the Cavity Mode Components of Raman Process and their Similarities with Atomic Collective Effects
11:00 – 11:30	Coffee Break	



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17 March 2016 SESSION: Computational Chemistry (CC) Symposium Biology (1) CHAIR: Takatsugu Hirokawa (ROOM 1)		
10:50 – 11:20	Akio Kitao	Parallel Cascade Selection Molecular Dynamics for Efficient Conformational Sampling and Free Energy Calculation of Proteins
11:20 – 11:50	Mariona Sodupe	Fluorescence Markers for Amyloid-β fibrils detection. Insights from computational approaches.
11:50 – 12:20	Masako Takasu	Mutual Positional Preference of IPMDH Proteins for Binding Studied by Coarse-grained Molecular Dynamics Simulation
12:20 – 12:50	Tanja van Mourik	Halogen bonding in molecules of biological interest
12:50 – 13:40	Lunch	



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17 March 2016 SESSION: Computational Chemistry (CC) Symposium Theory (1) CHAIR: Takahito Nakajima (ROOM 2)		
10:50 – 11:20	António Varandas	From CBS extrapolation to accurate potentials to quantum reaction dynamics
11:20 – 11:50	Hiroshi Teramoto	Classification of Electron Energy Level Crossings in terms of the Theory of Singularities and Analysis of Non-Adiabatic Transitions around the Crossings
11:50 – 12:20	Alessandro Genoni	New Insights and Perspectives in the Quest for “Experimental” Wave Functions
12:20 – 12:50	Naoum Bacalis	If an excited wave function is close to the exact but lies slightly below it, is it reliable?
12:50 – 13:40	Lunch	



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17 March 2016 SESSION: Pattern Recognition in Digital Images CHAIR: Selene Solorza Calderón (ROOM 3)		
11:30 – 12:00	Rodrigo Vélez-Rábago, Selene Solorza-Calderón, and Adina Jordan-Aramburo	Digital Image Pattern Recognition System Using Normalized Fourier Transform and Normalized Analytical Fourier-Mellin Transform
12:00 – 12:30	Carolina Barajas-García, Selene Solorza-Calderón, and Josué Álvarez-Borrego	Rotation, Scale and Translation Invariant Pattern Recognition System for Color Images
12:30 – 13:00	Perla Karina Barba-Rojo, Selene Solorza-Calderón, and Antonio González-Fernández	Pattern Recognition of Laminated Sediments Methodology
13:00 – 13:30	Claudia A. Vidales-Basurto, Josué Álvarez-Borrego, and José L. Poom-Medina	Invited Talk: A non- Gaussian Probability Analysis from the Sea Glitter Pattern
Lunch Break		



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17 March 2016		
SESSION: Computational Chemistry (CC) Symposium		
Materials (1), Surface, Solid		
CHAIR: Per-Olof Åstrand		
(ROOM 1)		
13:40 – 14:10	Wilson Agerico Diño	Surface as a Playground for Studying Gas-Surface Reaction Dynamics - From Elementary Dynamical Processes to Directed Materials Design -
14:10 – 14:40	Alexander F. Sax	On the role of adhesive forces in interface stability
14:40 – 15:10	Dennis Salahub	Multiscale Modeling of Chemical Reactions in Complex Environments
15:10 – 15:40	Andreas Grüneis	Towards Efficient Coupled Cluster Theories for Solids
15:40 – 16:00	Coffee Break	



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17 March 2016 SESSION: Computational Chemistry (CC) Symposium Theory (2) CHAIR: Andrei L. Tchougreeff (ROOM 2)		
13:40 – 14:10	Stefan Grimme	Simplified quantum chemical methods for consistent structures and energies of large systems
14:10 – 14:40	Alex Borgoo	Approximate orbital-free non-interacting kinetic energy density functionals from density scaling
14:40 – 15:10	Hiroyuki Nakashima	Solving the Schrödinger equations of interstellar molecules
15:10 – 15:40	Hiroshi Ishida	Spin-orbit interactions at solid surfaces studied by the embedded Green's function technique
15:40 – 16:00	Coffee Break	



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17 March 2016 SESSION: Computational Chemistry (CC) Symposium Materials (2), Dynamics CHAIR: Dennis Salahub (ROOM 1)		
16:00 – 16:30	Stephan Irle	Molecular Dynamics in Computational Materials Sciences: From the Study of Nanostructure Formation to the Design of Fluorescent Dyes
16:30 – 17:00	Akira Nakayama	First-principles simulations of oxygen vacancy transport at the metal/metal-oxide interface
17:00 – 17:30	Tomokazu Yasuike	Unified treatment of photo-induced adsorbate dynamics by an open-system approach for molecules interacting with environments
17:30 – 18:00	Sergei F. Vyboishchikov	Si···H···Si and H···Si···H interactions: structure and dynamics
18:00 – 18:30	Gabriel Hanna	Self-consistent transition filtering for efficient calculations of observables via mixed quantum-classical Liouville dynamics
18:30 – 20:00	Dinner	



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17 March 2016 SESSION: Computational Chemistry (CC) Symposium Inorganics (1), Magnetism CHAIR: Vincent Robert (ROOM 2)		
16:00 – 16:30	Taku Tsuchiya	Density Functional Computations in Earth and Planetary Physics
16:30 – 17:00	Juan Novoa	Modeling (and rationalizing) magnetic bistability in crystals of purely-organic radicals
17:00 – 17:30	Nina P. Gritsan	Magnetic properties of 4f- and 5d-metal complexes with redox-active ligands: the high-level ab initio calculations with non-perturbative account of spin-orbit coupling
17:30 – 18:00	Alexey Timoshkin	Computational studies of oligomeric 13-15 inorganic rings and cages
18:00 – 18:30	Tamotsu Inabe	Physical properties of the as-grown organic-inorganic hybrid perovskite semiconductors
18:30 – 19:00	Nathalie Guihéry	High-Spin Molecules resulting from the Double Exchange Mechanism and Magnetic and Transport Properties of Extended Double Exchange extended chains
19:00 – 20:00	Dinner	



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17 March 2016 SESSION: Computational Statistical Methods CHAIR: Frederico Caeiro (ROOM 3)		
15:00 – 15:25	<u>Flavius Guias</u>	Improving the stochastic direct simulation method with applications to evolution partial differential equations
15:25 – 15:50	<u>Dora Prata Gomes,</u> Inês Jorge Sequeira, Carlos Figueired, José Rueff and Aldina Brás	The human chromosomal fragile sites more involved in constitutional deletions and duplications - a statistical assessment
15:50 – 16:15	<u>Ayana Mateus,</u> Frederico Caeiro, Dora Prata Gomes and Inês Jorge Sequeira	Statistical Analysis of Extreme River Flows
16:15 – 16:40	<u>Frederico Caeiro,</u> Filipe J. Marques, AyanaMateus and Serra Atal	A note on the Jackson Exponentiality Test
16:40 – 17:00	<u>Ivanilda Cabral,</u> <u>Frederico Caeiro</u> and M. Ivette Gomes	Reduced Bias Hill estimators



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<p>17 March 2016</p> <p>SESSION: GENERAL SESSION II</p> <p>CHAIR: A. A. Kuleshov</p> <p>(ROOM 4)</p>		
<p>15:00 – 15:30</p>	<p><i>D. V. Alexandrov, I. V. Alexandrova, A. A. Ivanov</i></p>	<p>On the Theory of Steady-State Crystallization with a Non-Equilibrium Mushy Layer</p>
<p>15:30 – 16:00</p>	<p><i>K. Belyaev, A. Kuleshov, I. Kirchner, N. Tuchkova</i></p>	<p>Numerical Experiments with MPI-ESM Coupled Atmosphere-Land-Ocean Model in Conjunction with Data Assimilations in Arctic Region</p>
<p>16:00 – 16:30</p>	<p><i>Maryam Shojaei, Ali Mahani</i></p>	<p>A Novel 2-Phase Reliability Improvement of Digital Circuits</p>
<p>16:30 – 17:00</p>	<p><i>V. A. Balashov, E. B. Savenkov and A. A. Kuleshov</i></p>	<p>Direct Numerical Simulation of a Fluid Flow in Core Samples Based on Quasi-Hydrodynamic Equations</p>
<p>Coffee Break</p>		



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17 March 2016 SESSION: Cyber physical systems CHAIR: Ali Mahani (ROOM 1)		
17:30 – 18:00	<u>S. Deniziak, A.</u> <u>Dzitkowski</u>	Task scheduling for high performance low power embedded computing
18:00 – 18:30	<u>y.s. kavian, m.</u> <u>Jelodar</u>	Hardware description of artificial bee colony algorithm for implementing on FPGA
18:30 – 19:00	<u>a. Mahani, m.</u> <u>Shojaei</u>	A novel two phase reliability improvement for digital circuits

20:00 – 22:00	Welcome Drink
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Posters (17:00 - 19:00) (Special Session <i>Logic Synthesis and Control Systems</i>)	
<u><i>Iwona Grobelna</i></u> <u><i>Michał Grobelny</i></u> <u><i>Łukasz Stefanowicz</i></u>	A rule-based approach to model checking of UML state machines
<u><i>Remigiusz Wiśniewski</i></u> <u><i>Iwona Grobelna</i></u> <u><i>Łukasz Stefanowicz</i></u>	Partial reconfiguration of concurrent logic controllers implemented in FPGA devices
<u><i>Łukasz Stefanowicz</i></u> <u><i>Iwona Grobelna</i></u>	Application of modified Martinez-Silva algorithm in determination of net cover
<u><i>Marcin Kubica</i></u> <u><i>Kania Dariusz</i></u> <u><i>Adam Opara</i></u>	Decomposition time effectiveness for various synthesis strategies dedicated to FPGA structures
<u><i>Józef Kulisz</i></u> <u><i>Radosław Nawrot</i></u> <u><i>Dariusz Kania</i></u>	Synthesis of energy-efficient counters implemented in PLD circuits
<u><i>Krzysztof Kajstura</i></u> <u><i>Dariusz Kania</i></u>	A Novel Low Power State Assignment Algorithm
<u><i>Adam Opara</i></u> <u><i>Marcin Kubica</i></u>	Decomposition synthesis strategy directed to FPGA with special MTBDD representation
<u><i>Michał Kobylecki</i></u> <u><i>Kania Dariusz</i></u>	Double-tick realization of binary control program
<u><i>Józef Kulisz</i></u>	State Assignment for Asynchronous FSMs with the use of the Incompatibility and Complement Graph
<u><i>Stanisław Deniziak</i></u> <u><i>Mariusz Wiśniewski</i></u> <u><i>Konrad Kurczyna</i></u>	FPGA-oriented synthesis of multivalued logical networks



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Poster (17:00 - 19:00) (Special Session <i>Computational Data Analysis and Numerical Methods</i>)	
<i>Fernando Carapau</i>	Specific shear-dependent viscoelastic third-grade fluid model
<i>Lev Ryashko, Irina Bashkirtseva, Evdokia Slepukhina and Sergei Fedotov</i>	Stochastic dynamics and chaos in the 3D Hindmarsh-Rose model
<i>Lev Ryashko and Alexander N. Pisarchik</i>	Analysis of Stochastic Ricker Model in a Zone of Neimark-Sacker Bifurcation
<i>Irina Bashkirtseva</i>	Controlling Stochastic Gas Discharge System Under Incomplete Information
<i>Irina Bashkirtseva, Darja Filippova and Alexander N. Pisarchik</i>	Noise-Induced Extinction in Bazykin-Berezovskaya Population Model
<i>Maria Grazia Bonelli, Mauro Ferrini and Andrea Manni</i>	Artificial Neural Networks Environmental Forecasting In Comparison With Multiple Linear Regression Technique: From Heavy Metals To Organic Micropollutants Screening In Agricultural Soils

Poster (17:00 - 19:00) (General Session)	
<i>F. KAYADIBI, S. SAGDINC AND S. ZOR</i>	QUANTUM CHEMICAL STUDIES ON THE CORROSION INHIBITION OF ACETYLSALICYLIC ACID (ASPIRIN) BY DENSITY FUNCTIONAL THEORY

END OF THE 1ST DAY



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Highlight Invited Lectures (1) & Organizer Lecture (2)		
CHAIR: Taku Onishi & Tokuei Sako		
(ROOM 1)		
08:30 – 09:00	Igor Zilberberg	DFT predictions for hydrogen atom transfer at the $[\text{FeO}]^{2+}$ group: a distinct activity of the oxyl state $\text{Fe}^{\text{III}}-\text{O}\bullet$
09:00 – 09:30	Kunio Awaga	Crossroads between Organic Electronics and Solid-State Electrochemistry
09:30 – 10:00	Paul Geerlings	Chemical Concepts from Density Functional Theory: Chemistry from the Linear Response Function
10:00 – 10:30	Tokuei Sako	Theoretical framework for light-matter interaction in finite quantum systems
10:30 – 10:50	Coffee Break	



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18 March 2016 SESSION 11: Biosystems' control and signal processing CHAIR: Gerasimos Rigatos (ROOM 2)		
09:00 – 09:30	<i>Gerasimos Rigatos</i>	Differential flatness properties and adaptive control of the hypothalamic-pituitary-adrenal axis model
09:30 – 10:00	<i>Gerasimos Rigatos</i>	Differential flatness properties and multivariable adaptive control of ovarian system dynamics
10:00 – 10:30	<i>Gerasimos Rigatos and Alexey Melkikh</i>	Flatness-based control in successive loops for stabilization of heart's electrical activity
10:30 – 11:00	<i>Gerasimos Rigatos, Pierluigi Siano, Dan Selisteanu and Radu Emil Precup</i>	An H-infinity approach to optimal control of oxygen and carbon dioxide contents in blood
11:00 – 11:30	Coffee Break	

18 March 2016 SESSION 11: Biosystems' control and signal processing CHAIR: Gerasimos Rigatos (ROOM 2)		
11:30 – 12:00	<i>Gerasimos Rigatos, Efthymia Rigatou and Nikolaos Zervos</i>	A nonlinear H-infinity approach to optimal control of the depth of anaesthesia
12:00 – 12:30	<i>Gerasimos Rigatos, Nikolaos Zervos and Alexey Melkikh</i>	A flatness-based control approach to drug infusion for cardiac function regulation



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18 March 2016 SESSION: MS Applied and theoretical research on masonry CHAIR: Gabriele Milani (ROOM 3)		
09:10 – 09:30	<i>Gabriele Milani, Rafael Shehu, Marco Valente</i>	Seismic vulnerability of leaning masonry towers located in Emilia-Romagna region, Italy: FE analyses of four case studies
09:30 – 9:50	<i>Gabriele Milani, Rafael Shehu, Marco Valente</i>	Effects of FRP application on the seismic response of a masonry church in Emilia-Romagna (Italy)
9:50 – 10:10	<i>Francesco Clementi, Andrea Nespeca, Stefano Lenci</i>	Seismic behavior of an Italian Renaissance Sanctuary: Damage assessment by numerical modelling
10:10-10:30	<i>Antonio Formisano, Nicola Chieffo, Dario Monaco, Francesco Fabbrocino</i>	On the influence of the aggregate condition on the vibration period of masonry buildings: a case study in the district of Naples
10:30 – 10:50	<i>Renato S. Olivito, Carmelo Scuro, Rosamaria Codispoti</i>	Static analysis of masonry kilns built with fictile tubules bricks
11:00 – 11:30	Coffee Break	



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18 March 2016		
SESSION: Computational Chemistry (CC) Symposium		
Honorary Lecture (2) & Highlight Invited Lectures (2)		
CHAIR: Taku Onishi & Tokuei Sako		
(ROOM 1)		
10:50 – 11:50	Honorary Lecture Wim C. Nieuwpoort	Fifty Years in and around Theoretical Chemistry, a personal account.
11:50 – 12:20	Pere Alemany	Continuous Symmetry Measures: Expanding the Language of Symmetry to Describe an Asymmetric World
12:20 – 12:50	Yuichi Shimakawa	Unusual A-site magnetism in cation ordered transition-metal oxides studied comprehensively by experiments and theoretical calculations
12:50 – 13:40 (14:10)	Lunch	



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18 March 2016 SESSION: MS Applied and theoretical research on masonry CHAIR: Gabriele Milani (ROOM 3)		
11:30 – 11:50	<i>Elisa Bertolesi, Gabriele Milani, Siro Casolo</i>	Non-linear dynamic analyses of 3D masonry structures by means of a homogenized rigid body and spring model (HRBSM)
11:50 – 12:10	<i>Elisa Bertolesi, Gabriele Milani, Carlo Poggi</i>	Non-linear homogenized and heterogeneous FE models for FRCM reinforced masonry walls in diagonal compression
12:10 – 12:30	<i>Giovanni Castellazzi, Antonio Maria D’Altria, Stefano de Miranda, Stefano Magagnini, Antonio M. Tralli</i>	On the seismic behavior of the main tower of San Felice sul Panaro (Italy) fortress
12:30 – 12:50	<i>Antonio Formisano, Nicola Chieffo, Bartolomeo Milo, Francesco Fabbrocino</i>	The influence of local mechanisms on large scale seismic vulnerability estimation of masonry building aggregates
12:50 – 13:10	<i>Roberta Fonti, Erwin Emmerling</i>	On the reading of the structural behavior of old masonry: the issue of the seismic assessment of Archeological ruin
Lunch Break		



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<p>18 March 2016</p> <p>SYMPOSIUM 23: International Symposium of Computational and Mathematical Modeling of Biologic and Medicine Targets</p> <p>CHAIR: Dilson Silva and Celia M. Cortez</p> <p>(ROOM 4)</p>		
<p>11:30 – 12:00</p>	<p><u>Dilson Silva</u></p>	<p>Computational Challenges in Modeling and Simulating Living Matter.</p>
<p>12:00 – 12:30</p>	<p><u>M. Clicia S.de Castro</u></p>	<p>Modeling Gene Regulatory Networks: A Network Simplification Algorithm.</p>
<p>12:30 – 13:00</p>	<p><u>Celia M. Cortez</u></p>	<p>Dynamics for the Storage Control of an Endocrine Gland: A Model for Adrenal Epinephrine.</p>
<p>13:00 – 13:30</p>	<p><u>Ethel Valdez</u></p>	<p>Modeling the Accessibility of the Interaction of Clonazepan to Albumins.</p>
<p>Lunch Break</p>		



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18 March 2016 SESSION: Computational Chemistry (CC) Symposium K-Computer, Materials (3), Organics & Catalyst CHAIR: Pere Alemany (ROOM 1)		
13:40 – 14:10	Takahito Nakajima	NTChem: Quantum Chemistry on K Computer
14:10 – 14:40	Takeo Hoshi	One-hundred-nm-scale electronic structure and transport calculations of organic polymers on the K supercomputer
14:40 – 15:10	Feliu Maseras	Computational enantioselective catalysis with DFT and DFT/MM methods
15:10 – 15:40	Masato Ohashi	Ni(0)-Catalyzed Enantio- and Diastereoselective Synthesis of Benzoxasiloles



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18 March 2016 SESSION: Computational Chemistry (CC) Symposium Biology (2) CHAIR: Akio Kitao (ROOM 2)		
14:10 – 14:40	Yukari Fujimoto	Immunomodulatory Microbial Components; Their Structures, Syntheses and Biological Functions
14:40 – 15:10	Takatsugu Hirokawa	Molecular modeling of GPCRs for accurate in silico screening
15:10 – 15:40	Sotaro Fuchigami	Computational study on slow dynamics of proteins
15:40 – 16:10	Michele Cascella	A Native Human Protein Nanoconstruct with Acquired Transcytotic Properties through Endothelial Barriers
16:10 – 16:30	Coffee Break	



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18 March 2016		
SESSION: Computational Chemistry (CC) Symposium		
Materials (4), Organics & Catalyst, Vibration		
CHAIR: Nina P. Gritsan		
(ROOM 1)		
16:30 – 17:00	Yasuchika Hasegawa	Luminescent lanthanide coordination polymers with 4f-4f transitions
17:00 – 17:30	Jun Terao	Synthesis of Functionalized Conductive Wires
17:30 – 18:00	Azusa Muraoka	Electronically excited states of carbazole modified phenylenes
18:00 – 18:30	Michael Deleuze	Mechanisms and Kinetics of the Oxidation Reactions of Naphthalene Initiated by Hydroxyl Radicals
18:30 – 19:00	Hajime Torii	New twist in the theories on the secondary structure dependence and hydration effect of the vibrational properties of peptides
19:00 – 19:30	Tetsuya Nanba	Catalysis of soot oxidation and characterization of Ag catalysts
19:30 – 20:30	Dinner	



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18 March 2016 SESSION: Computational Chemistry (CC) Symposium Photo-chemistry, Cross Section CHAIR: Tokuei Sako (ROOM 2)		
16:30 – 17:00	Yasuhiro Ohshima	High-Resolution Spatiotemporal Imaging of Molecular Rotational Wave Packets
17:00 – 17:30	Reika Kanya	Laser-assisted elastic electron scattering by light-dressed Xe in intense laser fields
17:30 – 18:00	Benoit Mignolet	Control of electronic dynamics visualized by angularly resolved photoelectron spectra in LiH, PENNA and C ₆₀
18:00 – 18:30	Erik Lötstedt	Efficient solution of the time-dependent Schrödinger equation: Factorized CI approximation in MCTDHF
18:30 – 19:00	Frank De Proft	Chemical Concepts from Quantum Chemistry: Applications in Catalysis and Inverse Design of Molecules with Optimal Properties
19:00 – 19:30	Masashi Kitajima	Cross sections for ultra-low-energy electron scattering from atoms and molecules
19:30 – 20:30	Dinner	



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18 March 2016 SESSION: GENERAL SESSION III CHAIR: Robert Černý (ROOM 3)		
15:00 – 15:30	<i>Dana Koňáková, Václav Kočí, Jaromír Žumár, Martin Keppert, Ondřej Holčapek, Eva Vejmelková and Robert Černý</i>	Effect of Heat and Moisture Transport and Storage Properties of Building Stones on the Hygrothermal Performance of Historical Building Envelopes
15:30 – 16:00	<i>Lukáš Fiala, Jiří Maděra, Eva Vejmelková and Robert Černý</i>	Modeling of Heat Evolution in Silicate Building Materials with Electrically Conductive Admixtures
16:00 – 16:30	<i>Jan Kočí, Jiří Maděra and Robert Černý</i>	Analysis of the Impact of Applied Climatic Data on the Computational Modelling of Frost Damage in Building Structures
16:30 – 17:00	<i>J. Madera, T. Koudelka and Jaroslav Kruis</i>	Hygro-thermo-mechanical modeling of transport phenomena in the surface layers of building envelopes
17:00 – 17:30	Coffee Break	



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15:00 – 15:30	<u>Bruno Viveiros</u>	Greenhouse Effect Simulation – An Educational Application.
15:30 – 16:00	<u>Raimunda N.Fortes</u>	In situ Assessment of Two Catfish Species (Pisces, Ariidae) to Evaluate Pollution in a Harbor.
16:00 – 16:30	<u>Felipe Thadeu</u>	Mathematical-Computational Modeling for Calculations Involved in the Stern-Volmer Theory.
16:30 – 17:00	<u>Carla P. M. Coura</u>	Serum Albumin and the Haloperidol Pharmacokinetics. Study Using a Computational Model.
17:00 – 17:30	Coffee Break	



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18 March 2016 SESSION: GENERAL SESSION IV CHAIR: P. Vafeas (ROOM 3)		
17:30 – 18:00	<i>SEÇKİN D. GÜNAY</i>	ALPHA PARTICLE DAMAGE IN URANIUM DIOXIDE: EFFECT ON RADIAL DISTRIBUTION FUNCTION
18:00 – 18:30	<i>C. Chr. Koutsoumaris, K. G. Eptaimeros, T. Zisis and G. J. Tsamasphyros</i>	A Straightforward Approach to Eringen's Nonlocal Elasticity Stress Model and Applications for Nanobeams
18:30 – 19:00	<i>G. J. Tsamasphyros and C. Chr. Koutsoumaris</i>	Mixed Nonlocal-Gradient Elastic Materials with Applications in Wave Propagation of Beams
19:00 – 19:30	<i>E. Georgantzios and A. C. Boucouvalas</i>	Transmission Line resonance technique for Eccentric Core Optical Fibers
19:30 – 20:00	<i>D. Logothetis, P. K. Papadopoulos, P. Svarnas and P. Vafeas</i>	Comparison of two electrohydrodynamic force models for the interaction between helium jet flow and an atmospheric-pressure "plasma jet"



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17:30 – 18:00	<u>M. Clicia S. de Castro</u>	A Guide to Parallel Execution of Sequence Alignment
18:00 – 18:30	<u>Rafael F. Soares</u>	The Influence of the Pentose's Pathway of the <i>Clostridium acetobutylicum</i> on the Production of Butanol: Insights from Mathematical Modeling.
18:30 – 19:00	<u>Victor C. Gomes</u>	Modeling the Interaction of the Carbamate Fungicide Maneb, with Bovine Albumin.
19:00 – 19:30	<u>Marilia A. Soares</u>	A Model for the Neural Control of Pineal Periodicity
19:30 – 20:00	<u>M. Clicia S. de Castro</u>	Simulation Step Size Analysis of a Whole-Cell Computational Model of Bacteria.
20:00 – 20:30	<u>Marilia A. Soares</u>	A Computational Solution to Analyze Hydrophobic Characteristics in Protein Chains.



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18 March 2016 SESSION: ICCMSE 2016 INVITED SPEAKER CHAIR: TBA (ROOM 1)		
20:30 – 21:30	Anthony C. Boucouvalas	Predicting Earthquakes in 2016: “20 Earthquakes in 16”

18 March 2016 SESSION: Computational Chemistry (CC) Symposium Poster (ROOM 1)		
21:30 – 22:30		

END OF THE 2ND DAY



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19 March 2016		
SESSION: Computational Chemistry (CC) Symposium		
Highlight Invited Lectures (3)		
CHAIR: Taku Onishi & Tokuei Sako		
(ROOM 1)		
08:30 – 09:00	Roman Krems	Statistical learning for molecular dynamics: applications of Gaussian Processes for improved predictions of molecular collision observables
09:00 – 09:30	Holger Braunschweig	Boron-Boron-Bonds: Unexpected Results and New Insights
09:30 – 10:00	Takanori Fukushima	Precision Molecular Self-Assembly beyond Nanometer Length Scale
10:00 – 10:30	Yoshitada Morikawa	First-principles Simulations of Catalytic Reactions in Crystal Growth and Etching Processes at Semiconductor Interfaces
10:30 – 10:50	Coffee Break	



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19 March 2016 SESSION: Computational Chemistry (CC) Symposium Honorary Lecture (3) & Highlight Invited Lectures (4) CHAIR: Taku Onishi & Tokuei Sako (ROOM 1)		
10:50 – 11:50	Honorary Lecture Robert A. Evarestov	Symmetry and First-principles Calculations of Inorganic Nanostructures
11:50 – 12:20	Per-Olof Åstrand	Metal clusters on carbon surfaces as catalysts: Molecular dynamics simulations and quantum chemical calculations
12:20 – 12:50	Andrei L. Tchougreeff	Babylonian vs Greek Quantum Chemistry
12:50 – 13:00	Photo of CC symposium	
13:00 – 14:00	Lunch	



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19 March 2016 SESSION: Computational Data Analysis and Numerical Methods CHAIR: Luís M. Grilo (ROOM 3)		
09:00 – 09:30	Maria José Varadinov	“Imbedding Linear Regressions in Models for Factor Crossing”
09:30 – 10:00	Cristina Dias	“ANOVA Like Analysis for Structured Families of Stochastic Matrices”
10:00 – 10:30	Filomena Teodoro	“Approximating a Nonlinear MTFDE”
10:30 – 11:00	Atanasov Todorov	New Allometric Laws, Theory, Methods and Models Describing Living Organisms, and Corresponding Scientific Results Received by these Laws, Methods and Models
19 March 2016 SESSION: GENERAL SESSION V CHAIR: Z. Kalogiratou (ROOM 4)		
09:00 – 09:30	<i>Z. Kalogiratou, Th. Monovasilis</i>	Trigonometrically Fitted Two Derivative Runge – Kutta Methods.
09:30 – 10:00	<i>Th. Monovasilis, Z. Kalogiratou</i>	Modified Two Step Hybrid Methods for Oscillatory Problems.
10:00 – 10:30	<i>Seung-Jun Hwang, Seung-Je Park and Joong-Hwan Baek</i>	Online Signature Recognition Using Principal Component Analysis and Artificial Neural Network
10:30 – 11:00	<i>Fethi Kadioğlu and Gülçin Tekin</i>	Dynamic Response of Visco- Elastic Plates
11:00 – 11:30	Coffee Break	



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19 March 2016 SESSION: GENERAL SESSION VI CHAIR: Victor Kireev (ROOM 4)		
11:30 – 12:00	<i>Alfred Davletbaev, Victor Kireev, Liana Kovaleva, Aleksey Zainullin and Rais Minnigalimov</i>	Cold Heavy Oil Production and Production by Radio-Frequency Electromagnetic Radiation: Comparative Numerical Study
12:00 – 12:30	<i>Slawomir Bąk, Radosław Czarnecki and Stanisław Deniziak</i>	Scheduling of Distributed Applications for High Performance Computing as a Service
12:30 – 13:00	<i>Suchinthra Rungpitaxmana and Saifon Chaturantabut</i>	Dimension Reduction for Systems with Parametrized Boundaries for Fisher's Equation
13:00 – 13:30	<i>Victor Kireev, Liana Kovaleva, Ivan Shrubkovskiy, and Rasul Zinnatullin</i>	Numerical Modeling of Electromagnetic Heating of a Liquid Flowing in a Pipeline

19 March 2016 SESSION: Computational Data Analysis and Numerical Methods CHAIR: Luís M. Grilo (ROOM 3)		
11:30 – 12:00	Eliana Costa e Silva	“Consumer Default Risk Assessment in a Banking Institution”
12:00 – 12:30	Aldina Correia	“MANOVA for distinguishing experts perceptions about entrepreneurship using NES data from GEM”
12:30 – 13:00	Luis Miguel Grilo	“ Individual control charts in paperboard industry”



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14:00 – 18:00	Central Excursion
20:30 – 23:00	Central Dinner

END OF THE 3RD DAY



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20 March 2016 SESSION: Computational Chemistry (CC) Symposium Highlight Invited Lectures (5) CHAIR: Taku Onishi & Tokuei Sako (ROOM 1)		
08:30 – 09:00	Vincenzo Aquilanti	A transition rate theory beyond Arrhenius and Eyring
09:00 – 09:30	Michael Anisimov	THE NUCLEATION RATE SURFACES DESIGN OVER DIAGRAM OF PHASE EQUILIBRIA AND THEIR APPLICATIONS FOR COMPUTATIONAL CHEMISTRY
09:30 – 10:00	Vincent Robert	Weak Bonds for Structure and Recognition : ab initio Inspections
10:00 – 10:30	Koichi Yamashita	Energy Alignment of Frontier Orbitals and Suppression of Charge Recombinations in P3HT/SWNT
10:30 – 10:50	Coffee Break	

20 March 2016 SESSION: GENERAL SESSION VII CHAIR: J. Albert (ROOM 2)		
09:00 – 09:30	<i>J. Albert</i>	Stochastic simulation of reaction subnetworks: exploiting synergy between the chemical master equation and the Gillespie algorithm.
09:30 – 10:00	<i>Yuna Noh and Yoonjin Yoon</i>	Tactical Traffic Control for Multiple AGV Systems based on Three Dimensional Space
10:00 – 10:30	<i>Lapka Piotr</i>	Comparison of different bioheat transfer models for assessment of burns injuries



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20 March 2016 Symposium on Computational Combustion CHAIRs: Lucia Russo and Paola Russo (ROOM 3)		
09:00 – 09:25	<i>Mario Barone, Simone Lombardi, Gaetano Continillo, Paolo Sementa, Bianca Maria Vaglieco</i>	Application of the Optical Flow Method for the Experimental Analysis of Turbulent Flame Propagation in a Transparent Engine
09:25 – 09:50	<i>Mario Barone, Nabiha Chaumeix, Andrea Comandini, Gaetano Continillo, Simone Lombardi, Damien Nativel</i>	Unsupervised Analysis of Experiments of Laminar Flame Propagation in a Spherical Enclosure
09:50 – 10:15	<i>Francesco Miccio</i>	Integrated Model of a Composite Propellant Rocket
10:15 – 10:40	<i>Constantinos Spiliotis and Lucia Russo</i>	Shifts and oscillations in a forest-grassland ecosystem affected by fire
10:40 – 11:05	<i>L. Marmo, E. Danzi, V. Puccia and L. Fiorentini</i>	Modeling of a large fire of a non-conventional roof photovoltaic plant
11:05 – 11:35	Coffee Break	



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20 March 2016 SESSION: Computational Chemistry (CC) Symposium Highlight Invited Lectures (6) CHAIR: Taku Onishi & Tokuei Sako (ROOM 1)		
10:50 – 11:20	Kenichi L. Ishikawa	Multielectron Dynamics in Intense Laser Fields
11:20 – 11:50	Katsuhiko Ariga	Energy efficient mechanical manipulation of molecular machines at interfaces <i>Hand-Operating Technology: World-Stupidest Challenge in Nanotechnology</i> <i>How can we manipulate molecular machines by our hands?</i>
11:50 – 12:20	Kohzo Ito	Slide-Ring Materials: Novel Concept for Flexible and Tough Polymers
12:20 – 13:10	Lunch	



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20 March 2016		
SESSION:		
CHAIR:		
(ROOM 3)		
11:35 – 12:00	<i>Joules Goulier, Katarzyna Bizon, Nabiha Chaumeix, Nicolas Meynet, and Gaetano Continillo</i>	Numerical Assessment of Accurate Measurements of Laminar Flame Speed
12:00 – 12:25	<i>Ivano Coccorullo, Paola Russo</i>	Jet fire consequence modelling for high pressure gas pipelines
12:25 – 12:50	<i>Lucia Russo, Paola Russo, Constantinos I. Siettos</i>	Mitigating Wildland Fire Hazard using Complex Network Centrality Measures
12:50 – 13:15	<i>K.G. Eptaimeros, C.Chr. Koutsoumaris, G.J. Tsamasphyros</i>	Nonlocal Integral elasticity analysis of nanobeams by employing finite element method
Lunch Break		



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20 March 2016 SESSION: Computational Chemistry (CC) Symposium Biology (3), Dynamics CHAIR: Michele Cascella (ROOM 1)		
13:10 – 13:40	Fernanda Duarte	Evolution Through Cooperativity in the Alkaline Phosphatase Superfamily
13:40 – 14:10	Takefumi Yamashita	Molecular Dynamics Simulation of biomolecules: Accuracy Improvement and Computational Conditions
14:10 – 14:40	Shinnosuke Kawai	Essential Dynamical Coordinates to Describe Molecular Systems in Condensed Phase
14:40 – 15:10	Norifumi Yamamoto	Protein Secondary Structure Principal Component Analysis: Hot Spot of Structural Ambivalence in Prion Protein
15:10 – 15:40	YounJoon Jung	Dynamic Heterogeneity in Room Temperature Ionic Liquids



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20 March 2016 SESSION: Computational Chemistry (CC) Symposium Hydrogen, Inorganics (2) CHAIR: Wilson Agerico Diño (ROOM 2)		
13:10 – 13:40	Masanori Tachikawa	Path integral simulation on muoniated acetone radical
13:40 – 14:10	Yoong-Kee Choe	First-principles molecular dynamics simulation study on polymer electrolyte membranes for fuel cell applications
14:10 – 14:40	Ioannis Kerkines	Designing Nonclassical Hydrogen Complexes: The case of $\text{Si}_2\text{F}_3(\text{H}_2)$
14:40 – 15:10	Anna Pomogaeva	Mechanisms of Hydrogen Release from Small Clusters of Lithium Amidoborane
15:10 – 15:40	Toshihiro Moriga	Control of Optical Properties of Perovskite-related Oxynitrides through Stoichiometries
15:40 – 16:10	Alex Domingo	Polarization induced metal–arene: a second order non-covalent interaction
16:10 – 16:30	Coffee Break	



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20 March 2016		
Symposium on Computational Combustion		
CHAIRs: Lucia Russo and Paola Russo		
(ROOM 3)		
15:00 – 15:30	L. Marmo, E. Danzi, V. Puccia and L. Fiorentini	Modeling of a large fire of a non- conventional roof photovoltaic plant

20 March 2016		
SESSION: Computational Chemistry (CC) Symposium		
Materials (6), Organics, Excited State		
CHAIR: Hiroyuki Teramae & Taku Onishi		
(ROOM 1)		
16:30 – 17:00	Takashi Sugimura	Solid Catalyst for Asymmetric Synthesis. Tartaric Acid-Modified Raney Nickel for Hydrogenation of β- Keto Esters
17:00 – 17:30	Hiroyuki Teramae	Hamiltonian algorithm and its application to the aromatic oxidative cyclization on N-methoxy-N- prenylbenzamide
17:30 – 18:00	John Herbert	Beyond TDDFT Using Only Single Excitations: Methods for Computational Studies of Excited States in Complex Systems
18:00 – 18:30	Yoshiaki Shoji	Electronic Structure and Reactivity of Unprecedented Two-Coordinate Boron Cation with C–B⁺–C Bonding
18:30 – 19:00	Yasunori Matsui	"Excited State C–C Bond Cleavage- Luminescence" of Methylenecyclopropanes and Related Theoretical Calculations



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20 March 2016 SESSION: Computational Chemistry (CC) Symposium Physical Chemistry CHAIR: Toshihiro Moriga (ROOM 2)		
16:30 – 17:00	Jun Tsuchiya	Elasticity of ice VIII and ice X under pressure.
17:00 – 17:30	Federico Palazzetti	Spherical and hyperspherical – harmonics representation of van der Waals aggregates.
17:30 – 18:00	Manabu Sugimoto	Electronic-Structure Informatics Using the First-Principles Molecular Dynamics Method: Application to Search for Active Sites on Heterogeneous Catalysts
18:00 – 18:20	Bui Van Pho	First-Principles Calculations of Initial Etching Process of SiC with Water Assisted by Platinum Catalyst
18:20 – 18:40	Elena Koblova	Quantum Chemical Calculations of Anion Complex $[B_{12}HX(CF_3)_{12-X}]^{2-}$ (X = 9 – 12)



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20 March 2016 SESSION: Computational Chemistry (CC) Symposium Short Oral Presentation for Poster CHAIR: Taku Tsuchiya (ROOM 2)	
19:10 – 19:35	Evgheni Jucov Keigo Saito Takahiko Yoshida Gil Gallegos Ai Ishohashi

END OF THE 4TH DAY
END OF THE CONFERENCE