



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

22 April 2017 SESSION: Computational Chemistry Symposium (1) Organizer lecture, Honorary lecture CHAIRS: Taku Onishi, Tokuei Sako (ROOM 1)		
08:30 – 08:40	Opening	
08:40 – 09:05	Taku Onishi	A theoretical study of covalent bonding formation related to helium
09:05 – 09:30	Tokuei Sako	Near-field effect in optically controlling simple quantum systems
09:30 – 10:20	Josef Paldus	Honorary lecture (50 min) Coupled Cluster Approaches are Alive and Well: A Biased Eyewitness Recount
10:20 – 10:40	Photograph, Coffee Break	



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

22 April 2017 SESSION: Numerical Modeling, Experimentation and Design Practice for Masonry Structures in Seismic Prone Areas CHAIR: F Clementi, A Formisano, G Milani (ROOM 3)		
09:00 – 09:15	<u>G. Stockdale</u> <u>G. Milani</u>	FE model predicting the increase in seismic resistance induced by the progressive FRP strengthening on already damaged masonry arches subjected to settlement
09:15 – 9:30	<u>A. Formisano</u> <u>G. Ciccone</u>	Large scale seismic vulnerability evaluation of masonry churches: an application in the historical centre of Naples
9:30 – 9:45	<u>E. Bertolesi</u> <u>G. Carozzi</u> <u>G. Milani</u> <u>C. Poggi</u>	Masonry arches retrofitted with FRP and FRCM: in situ experimental tests and advanced FE simulations
9:45 – 10:00	<u>C. Clementi</u> <u>F. Clementi</u> <u>S. Lenci</u>	Nonlinear analyses and failure patterns of typical masonry school buildings in the epicentral zone of the 2016 Italian earthquakes
10:00 – 10:15	<u>A. Formisano</u> <u>E. J. Dessi</u> <u>R. Landolfo</u>	Mechanical-physical experimental tests on adobe bricks reinforced with hemp fibres
10:15 – 10:30	<u>Olivito RS</u> <u>Codispoti RM</u> <u>Scurio C</u>	Seismic analysis for masonry construction: different schematization methods of masonry walls
10:30-10:45	<u>N Grillanda</u> <u>F Manconi</u> <u>F Stochino</u> <u>A Cazzani</u> <u>F Bondi</u> <u>A Chiozzi</u> <u>A Tralli</u>	On the Analysis of the Stellar Vault of Santa Maria del Monte in Cagliari
11:00 – 11:30	Coffee Break	



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

22 April 2017 SESSION 37: GIS, Statistics and Remote Sensing Technologies for River Valleys Development CHAIR: Michał Habel (ROOM 4)		
09:00 – 09:30	<u>Hubert Rabant,</u> <i>Dawid Szatten and</i> <i>Grzegorz Nadolny</i>	The Analysis of Inland Water Transport on Technically Developed Polish Section of the E70 Waterway Using GIS Tools in the Years 2005-2014
09:30 – 10:00	<u>Grzegorz Nadolny,</u> <i>Hubert Rabant and</i> <i>Dawid Szatten</i>	Application of GIS Tools in Determining the Navigability of Waterways
10:00 – 10:30	<u>Dawid Szatten,</u> <i>Hubert Rabant and</i> <i>Grzegorz Nadolny</i>	The Use of GIS Tools in Determining the Intensity of Meandering of Rivers Based on the Example of Noteć River (Poland)
10:30 – 11:00	<u>Magdalena Matysik</u>	Impact of Land Development on Shaping Catchment Runoff Under the Influence of Mining Activity
11:00 – 11:30	Coffee Break	



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

22 April 2017 SESSION: 1st Symposium on Computational Simulation and Experimental Analysis of Hygrothermal Phenomena in Historical Building Envelopes CHAIR: Tomáš Koudelka (ROOM 5)		
09:00 – 09:20	<u>Miloš Jerman</u> , <u>Miloš Solař</u> , and <u>Robert Černý</u>	Interior thermal insulation systems for historical building envelopes
09:20 – 9:40	<u>Jiří Maděra</u> , <u>Václav Kočí</u> , <u>Jan Kočí</u> , and <u>Robert Černý</u>	Physical and Mathematical Models of Hygrothermal Processes in Historical Building Envelopes
09:40 – 10:00	<u>Václav Kočí</u> , <u>Jiří Maděra</u> , <u>Martin Keppert</u> , and <u>Robert Černý</u>	Hygrothermal Analysis of Surface Layers of Historical Masonry
10:00 – 10:20	<u>Václav Kočí</u> , <u>Miloš Jerman</u> , <u>Lukáš Fiala</u> , and <u>Robert Černý</u>	Effect of Hygric and Thermal Properties of Connecting Layers on the Performance of Interior Thermal Insulation Systems
10:20 – 10:40	<u>Miloš Jerman</u> and <u>Robert Černý</u>	Thermal insulation materials for inside applications: hygric and thermal properties
10:40 – 11:00	<u>T. Krejčí</u> , <u>J. Kruis</u> , <u>T. Koudelka</u> , and <u>M. Šejnoha</u>	Processor farming in two-level analysis of historical bridge
11:00 – 11:30	Coffee Break	



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

22 April 2017 SESSION: Computational Chemistry Symposium (2) Theory (1) CHAIR: Andrei Tchougréeff (ROOM 1)		
10:40 – 11:05	Ronnie Kosloff	Semi-global approach for propagation of the time-dependent Schrödinger equation for time-dependent and nonlinear problems
11:05 – 11:30	Matthias Ernzerhof	Developing new models for the exchange-correlation hole to better approximate the exchange-correlation energy
11:30 – 11:55	Alex Borgoo	Magnetic fields in Kohn-Sham theory: molecular properties and the adiabatic connection for a B-dependent exchange-correlation functional
11:55 – 12:20	Muneaki Kamiya	Development of two-component relativistic time-dependent density functional theory with spin-orbit interaction
12:20 – 12:45	Nektarios N. Lathiotakis	Approximating the many-electron problem with functionals of the one-body reduced density matrix
12:45 – 13:10	Ioannis S.K. Kerkines	The fascinating ground state structure of SF_6^-. Too close to call?
Lunch Break		



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

22 April 2017 SESSION: Computational Chemistry Symposium (3) Materials (1) CHAIR: Dennis Salahub (ROOM 2)		
10:40 – 11:05	Wilson Agerico Diño	Surface as a Playground for Studying Gas-Surface Reaction Dynamics - increasing the ortho-para H₂ conversion yield via molecular orientation, a case study -
11:05 – 11:30	Hiroshi Nakanishi	Inter-element Fusion Design for creating high performance material functions
11:30 – 11:55	Susumu Yanagisawa	Determination of geometric and electronic structures of organic crystals from first principles: Role of the molecular configuration on the electronic structure
11:55 – 12:20	Michihisa Koyama	Applications of Computational Chemistry to Fuel Cell Electrodes
12:20 – 12:45	Tetsuya Yamamoto	Codoping method toward the resolution of the doping-asymmetry for wide-gap semiconductors
12:45 – 13:10	Darya Alontseva	Precision Application of Powder Coating Multifunctional Systems for Protecting the Surfaces of Industrial Products
Lunch Break		



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

22 April 2017 SESSION: CHAIR: F Clementi, A Formisano, G Milani (ROOM 3)		
11:30 – 11:45	<u>LC Silva</u> <u>G Milani</u> <u>PB Lourenço</u>	Derivation of the out-of-plane behavior on an English bond masonry wall through homogenization strategies
11:45 – 12:00	<u>Tiberti S</u> <u>Milani G</u> <u>Codispoti R</u> <u>Scuro C</u> <u>Olivito RS</u>	Fictile tubules masonry arches: advanced FE homogenized computations
12:00 – 12:15	<u>Milani G</u> <u>Shehu R</u> <u>Valente M</u>	Comparison among different retrofitting strategies for the vulnerability reduction of masonry bell towers
12:15 – 12:30	<u>Habieb H</u> <u>Milani G</u> <u>Tavio T</u> <u>Milani F</u>	A low cost rubber seismic isolation system for new masonry residential buildings in developing countries
12:30 -12:45	<u>F Clementi</u> <u>A Pierdicca</u> <u>F Catinari</u> <u>S Lenci</u>	Identification and calibration of the structural model of historical masonry building damaged during the 2016 Italian earthquakes: The case study of Palazzo del Podestà in Montelupone
Lunch Break		



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

22 April 2017 SESSION 37: GIS, Statistics and Remote Sensing Technologies for River Valleys Development CHAIR: Ireneusz Malik (ROOM 4)		
11:30 – 12:00	<i><u>Michał Habel,</u></i> <i><u>Zygmunt Babiński</u></i> <i>and Dawid Szatten</i>	Using GIS to Appraise Structural Control of River Bottom Near Hydrotechnical Objects on the Alluvial Rivers
12:00 – 12:30	<i>Damian Absalon</i> <i>and <u>Magdalena</u></i> <i><u>Matysik</u></i>	Effects of Renaturation of the River Valley Transformed as a Result of Mining Activity - the Szarlejka River Case Study
12:30 – 13:00	<i><u>Damian Absalon,</u></i> <i><u>Paweł Kryszczuk</u></i> <i>and Paweł</i> <i>Rutkiewicz</i>	Changes in Water Quality Along the Course of a River - Classic Monitoring Versus Patrol Monitoring
13:00 – 13:30	<i><u>Michał Habel and</u></i> <i><u>Zygmunt Babiński</u></i>	A Comparison of Research Approaches in Estimation of Volume Changes of a Bed Load Transport Along a River Course on the Example of a Large Lowland River
Lunch Break		



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

22 April 2017 SESSION: 1st Symposium on Computational Simulation and Experimental Analysis of Hygrothermal Phenomena in Historical Building Envelopes CHAIR: Tomáš Krejčí (ROOM 5)		
11:30 – 11:50	<i><u>Tomáš Koudelka</u> and <u>Tomáš Krejčí</u></i>	Two-scale framework for coupled problems
11:50 – 12:10	<i><u>Magdalena Doleželová</u> and <u>Alena Vimmrová</u></i>	Optimization of the Gypsum-Based Materials by the Sequential Simplex Method
12:10 – 12:30	<i><u>Magdaléna Doleželová</u>, <u>Monika Čáchová</u>, <u>Lenka Scheinherrová</u>, and <u>Martin Keppert</u></i>	Time Evolution of Pore System in Lime – Pozzolana Composites
12:30 – 12:50	<i><u>Jan Kočí</u>, <u>Jiří Maděra</u>, <u>Václav Kočí</u>, <u>Zuzana Hlaváčová</u>, and <u>Robert Černý</u></i>	Thawing of Ice in Porous Space of Building Materials: Experimental Monitoring and Computational Modelling
Lunch Break		



ICCMSE 2017
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21-25 April 2017

22 April 2017 SESSION: Computational Chemistry Symposium (4) Spintronics: from fundamentals to next generation memory devices(1) CHAIRS: Andrei Kirilyuk, Masaki Mizuguchi (ROOM 1)		
14:00 – 14:25	T. Ono	Current-induced magnetic domain wall motion
14:25 – 14:50	Arata Tsukamoto	Ultrafast light manipulation and detection of spin dependent phenomena
14:50 – 15:15	R. L. Stamps	Numerical Models of dynamics in Artificial Spin Ice
15:15 – 15:40	S. Ohya	Spin transistors and novel spin-related quantum phenomena obtained with ferromagnetic semiconductors
15:40 – 16:05	Shuichi Murakami	Berry curvature, Hall effect and topological edge modes of magnons
16:05 – 16:30	S. Chadov	Room temperature tetragonal noncollinear Heusler antiferromagnet Pt ₂ MnGa
Coffee Break		



ICCMSE 2017
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21-25 April 2017

Change of Schedule

22 April 2017 SESSION: Computational Chemistry Symposium (5) Dynamics(1) CHAIRS: Akihiro Morita, Noam Agmon (ROOM 2)		
14:00 – 14:25	Akihiro Morita	Molecular Theory of Ion Transport at Oil-Water Interfaces
14:25 – 14:50	Noam Agmon	Infrared spectra of $M^+(H_2O)_4$ clusters (M=Na, H): Not simply the most stable isomer
14:50 – 15:15	Gabriel Hanna	A model platform for rapid, robust, directed, and long-range vibrational energy transport: Insights from a mixed quantum-classical study of a one-dimensional molecular chain
15:15 – 15:40	Yoong-Kee Choe	First-principles molecular dynamics simulation study on electrolytes for use in redox flow battery
15:40 – 16:05	Hiroki Nada	Molecular dynamics simulation studies on the mechanism of crystal morphology control by additives
Coffee Break		



ICCMSE 2017
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21-25 April 2017

22 April 2017

**SESSION: Modern information technology as an Instrument used in
Sport, Tourism and Recreation to Build a Healthy Society**

**CHAIR: drMirosławaSzark-Eckardt and
doc. PaedDr. Elena Bendíková
(ROOM 3)**

15:00 – 15:15	Michalina Kuska, Hanna Żukowska	Smartphone Applications as a Source of Motivation for Engaging in Physical Activity
15:15 – 15:30	Wiesława Pilewska, Krzysztof Buśko, Pantelis Theodoros Nikolaidis	Measuring the force of punches using a accelerometric punching bag – relationship between force of punches and power of jump – an example of application of the modern information technology in sport
15:30 – 15:45	Mirosława Szark-Eckardt	GPS as a Tool used in Tourism as Illustrated by Selected Mobile Applications
15:45 – 16:00	Jolanta G. Zuzda, Wiesław Półjanowicz, Robert Latosiewicz, Piotr Borkowski, Mirosław Bierkus, Owidiusz Moska	Innovative e-portal for prevention and therapeutic program for treatment of obesity and overweight in health-tourism
16:00 – 16:15	Jolanta Grażyna Zuzda, Piotr Borkowski, Justyna Popławska, Robert Latosiewicz, Eleonora Moska	Computer Methods in Designing Tourist Equipment for People with Disabilities
16:15 – 16:30	Marcin Pasek, Barbara Wilk, Ewa Kupcewicz, Monika Opanowska, Remigiusz Drózdź, Jacek Olszewski-Strzyżowski, Wojciech Sakłak, Artur Ziółkowski	Modern Information Technology as a Factor Supporting Participation in Physical Culture of a Contemporary Man
16:30 – 16:45	Wioletta Lubkowska	The potential of computer software that supports the diagnosis of workplace ergonomics in shaping health awareness



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

22 April 2017 SESSION 37: GIS, Statistics and Remote Sensing Technologies for River Valleys Development CHAIR: Magdalena Matysik (ROOM 4)		
15:00 – 15:30	<u>Ireneusz Malik,</u> <u>Małgorzata</u> <u>Wistuba, Yongbo</u> <u>Tie, Piotr Owczarek,</u> <u>Beata Woskowicz-</u> <u>Ślęzak, Katarzyna</u> <u>Łuszczynska and</u> <u>Damian Absalon</u>	A Tree-Ring and GIS Assessment of Mass-Movement Hazard in the Moxi Basin (Sichuan, China)
15:30 – 16:00	<u>Małgorzata</u> <u>Wistuba,</u> <u>Aleksandra Osika,</u> <u>Ireneusz Malik and</u> <u>Katarzyna</u> <u>Łuszczynska</u>	Reconstructing the Evolution of Hillslope-Valley Topography Based on DTM from Airborne LiDAR (Central Sudetes, Poland)
16:00 – 16:30	<u>Paweł Rutkiewicz,</u> <u>Ireneusz Malik,</u> <u>Daniel Gawior,</u> <u>Beata Woskowicz-</u> <u>Ślęzak, Paweł</u> <u>Kryszczuk</u>	Geomorphic Record of Historical Ferrous Metallurgy in Mała Panew and Czarna River Valleys (Poland) – analysis of DEM from Airborne LiDAR
16:30 – 17:00	<u>Katarzyna</u> <u>Łuszczynska,</u> <u>Małgorzata</u> <u>Wistuba, Ireneusz</u> <u>Malik</u>	Landslide Activity as a Threat to Infrastructure in River Valleys – an Example from Outer Western Carpathians (Poland)
17:00 – 17:30	Coffee Break	



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

22 April 2017 SESSION: Fluid Dynamics CHAIR: Constantin TANASA (ROOM 5)		
15:00 – 15:30	Sergey Molev, Vladimir Podaruev and Alexey Troshin	Fractional Time Stepping for Unsteady Engineering Calculations on Parallel Computer Systems
15:30 – 16:00	N. Nikolov, St. Radev and S. Tabakova	Pulsatile Blood Flow in Elastic Artery with Model Aneurysm
16:00 – 16:30	Sergey Mikhaylov, Alexander Morozov, Vladimir Podaruev and Alexey Troshin	A High-Order Solver for Aerodynamic Flow Simulations and Comparison of Different Numerical Schemes
16:30 – 17:00	Constantin TANASA, Tiberiu CIOCAN and Sebastian MUNTEAN	Numerical Assessment of Pulsating Water Jet in the Conical Diffusers
17:00 – 17:30	Said Urmancheev and Victor Kireev	The Transient Flow of Liquid with Non-Monotonous Temperature Dependent Viscosity in a Plane Channel



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

22 April 2017 SESSION: Computational Chemistry Symposium (6) Spintronics: from fundamentals to next generation memory devices(2) CHAIRS: Shuichi Murakami, Arata Tsukamoto (ROOM 1)		
16:50 – 17:15	Erik Tellgren	Quantum-chemical calculations on molecules in strong magnetic fields
17:15 – 17:40	Masaki Mizuguchi	Spin caloritronics in ordered alloy materials
17:40 – 18:05	A. Starikova	Computational design of dinuclear cobalt complexes with redox-active tetradentate ligands for molecular electronics and spintronics
18:05 – 18:30	Andrei Kirilyuk	Magnetization Dynamics and Switching by Laser Pulses
18:30 – 18:55	Emi Minamitani	Mechanically induced quantum phase transition in a single molecule
18:55 – 19:15 (20 min)	J. Ingla-Aynés	Directional control of spin currents and long spin relaxation lengths in hexagonal Boron Nitride encapsulated bilayer graphene
Dinner		



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

22 April 2017 SESSION: Computational Chemistry Symposium (7) Biology CHAIRS: Masako Takasu, Jean-Philip Piquemal (ROOM 2)		
16:50 – 17:15	Masako Takasu	Structure and Hydrogen Bonds of γS-crystallin and γS-G18V Studied by Molecular Dynamics Simulation
17:15 – 17:40	Jean-Philip Piquemal	TINKER-HP: Massively parallel simulations of biosystems on thousands of cores using new generation polarizable force fields
17:40 – 18:05	Hiroyuki Teramae	An Attempt at Ab Initio Crystal Orbital Calculation of Electronic Structure of B-type model-DNA
18:05 – 18:30	Toyokazu Ishida	Computational modeling of carbohydrate recognition in proteins
18:30 – 18:55	Toshiyuki Hirano	Study of High-Performance Canonical Molecular Orbitals Calculation for Proteins
18:55 – 19:20	Takefumi Yamashita	A Molecular Dynamics Study on Antigen-Antibody Recognition
Dinner		



ICCMSE 2017

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21-25 April 2017**

22 April 2017

**SESSION: Modern information technology as an
Instrument used in Sport, Tourism and Recreation to
Build a Healthy Society**

**CHAIR: drMirośławaSzark-Eckardt and
doc. PaedDr. Elena Bendíková
(ROOM 3)**

17:30 – 17:45	Michalina Kuska, Beata Augustyńska, Emilia Mikołajewska, Dariusz Mikołajewski	M-tourism As Increasing Trend Within Current Tourism And Recreation - Polish And International Experience
17:45 – 18:00	doc. PaedDr. Elena Bendíková	TBA
18:00 – 18:45	DISCUSSION	

22 April 2017

SESSION: Metamaterials

**CHAIR: T. Gric
(ROOM 3)**

18:45 – 19:15	<u><i>O. Hess</i></u> <i>(Invited speaker)</i>	Active and chiral nanoplasmonic metamaterials
19:15 – 19:45	<u><i>O. Hess</i></u> <i>(Invited speaker)</i>	Active and chiral nanoplasmonic metamaterials
19:45 – 20:15	<u><i>O. Hess</i></u> <i>(Invited speaker)</i>	Active and chiral nanoplasmonic metamaterials
20:15 – 20:45	<u><i>T. Gric</i></u>	Positional irregularities in metamaterials



ICCMSE 2017
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21-25 April 2017

22 April 2017 SESSION 37: GIS, Statistics and Remote Sensing Technologies for River Valleys Development CHAIR: Damian Absalon (ROOM 4)		
17:30 – 18:00	<i>Daniel Gawior, Paweł Rutkiewicz, Ireneusz Malik and <u>Małgorzat Wistuba</u></i>	Contribution to Understanding the Post-mining Landscape – Application of Airborn LiDAR and Historical Maps at the example from Silesian Upland (Poland)
18:00 – 18:30	<i><u>Danuta Szumińska,</u> Daniel Pakuła and Sebastian Czapiewski</i>	Transformation of the Wda River Channel in the 20th Century (the Tuchola Pinewoods, Poland)
18:30 – 19:00	<i><u>Danuta Szumińska,</u> Sebastian Czapiewski and Katarzyna Machowiak</i>	Morphological Diversification of the Valley Bottom with Reference to Lithological Conditions (Orkhon River, Mongolia)
19:00 – 19:30	<i><u>Barbara Waldon-</u> <u>Rudzonek</u></i>	Comparison of plant cover of river valley fragments by using GIS tools and multivariate analysis
19:30 – 20:00	<i><u>Beata Woskowicz-</u> <u>Ślęzak</u>, Albert Ślęzak, Daniel Gawior and Paweł Rutkiewicz</i>	Geomorphological Record of the Soła River Channel Dynamics in the Light of a DTM Based on LiDAR Data (Western Carpathian Foreland, Poland)



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

22 April 2017 SESSION: Advanced Computational Methods in Vibration Signals CHAIR: Ya-juan Xue (ROOM 5)		
17:30 – 18:00	Huimin ZHANG Institute of Solid Mechanics, Beihang University (BUAA), Beijing, China	Fourth-order Newmark Method for Structural Dynamics Analysis
18:00 – 18:30	Dingding ZHANG Hospital of University of Electronic Science and Technology and Sichuan Provincial People's Hospital, Sichuan, China	Evaluation the COL9A2 Gene with High Myopia
18:30 – 19:00	Yujia Lu Chengdu University of Technology, Chengdu, China	Seismic Fracture Detection of Shale Gas Reservoir in Longmaxi Formation, Sichuan Basin, China
19:00 – 19:30	Ya-juan Xue School of Communication Engineering, Chengdu University of Information Technology, Chengdu, China	Application of CEEMD-based Attenuation Estimation and Wavelet-based Cepstrum Decomposition in Shale Gas Reservoir Characterization
19:30 – 20:00	Xu-dong Jiang College of Geophysics, Chengdu University of Technology, Chengdu, China	Prediction of TOC Based on Pre-stack Inversion and Double Hidden layer BP Neural Network



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

22 April 2017 SESSION: ICCMSE 2017 INVITED SPEAKER CHAIR: Taku Onishi (ROOM 1)		
20:30 – 21:20	Paul Mezey	The Holographic Electron Density Theorem, De- quantization, Re- quantization, and Nuclear Charge Space Extrapolations of the Universal Molecule Model

21:30 – 22:30	Welcome drink & Poster of Computational Chemistry Symposium
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END OF THE 1ST DAY



ICCMSE 2017
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21-25 April 2017

23 April 2017 SESSION: Computational Chemistry Symposium (8) Keynote lecture, Highlight lecture CHAIRS: Vincent Robert, Teruo Ono (ROOM 1)		
08:30 – 09:10	J.-P.Malrieu	Keynote lecture (40 min) In search of reference-independent excitation amplitudes in Multi-Reference methods: new MR-PT-2 and MR-CC algorithms
09:10 – 09:35	Nathalie Guihéry	Extraction of Hubbard and Heisenberg Interactions from Broken Symmetry DFT Calculations : impact of the HFX on the accuracy of the calculated values
09:35 – 10:00	Sadamichi Maekawa	Spin Transport in Spintronics
10:00 – 10:25	Eiji Saitoh	Spin Current Generators
Lunch Break		



ICCMSE 2017
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21-25 April 2017

23 April 2017 SESSION: Computational Data Analysis and Numerical Methods CHAIR: Luis M. Grilo (ROOM 2)		
09:00 – 09:30	Henrique Pinho	Computation of Bubble Mean Diameters using Probability Distribution Function
09:30 – 10:00	Alessandro Barbiero	A bivariate geometric distribution with positive or negative correlation
10:00 – 10:30	Eliana Costa e Silva	Experts' perceptions on the Entrepreneurial Framework Conditions
10:30 – 11:00	Fátima Almeida	Mechanical Properties of PA6/PP Compatibilized Nanocomposites Using a Twin Screw Extruder
11:00 – 11:30	Coffee Break	



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
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23 April 2017 Symposium on Computational Methods in Economics and Nature Use CHAIR: Aleksandr N. Medvedev (ROOM 3)		
09:00 – 09:20	Anna Rylova	Modeling of the Interest Rate Policy of the Central Bank of Russia
09:20 – 09:40	Olga Zvereva	Imbalance Detection in a Manufacturing System: An Agent-Based Model Usage
09:40 – 10:00	Olga Zvereva	Mitigation of Short-term Disturbance Negative Impacts in the Agent-Based Model of a Production Companies Network
10:00 - 10:20	Sergey Porshnev	Identification of Pulsating Combustion Modes of Gaseous Fuel
10:20 - 10:40	Sergey Porshnev	On Application of the SSA Method in the Pulsating Combustion Studies
10:40 – 11:00	Ivan Berg	Machine Learning in Smart Home Control Systems - Algorithms and New Opportunities
11:00 – 11:30	Coffee Break	



ICCMSE 2017
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21-25 April 2017

23 April 2017 2th Symposium on Computational Combustion CHAIRs: Lucia Russo and Gaetano Continillo (ROOM 4)		
09:00 – 10:00 Topical talk	<u>Giancarlo Sorrentino</u> , Istituto di Ricerche sulla Combustione, CNR, Italy	Modeling challenges of distributed combustion regimes
10:00 – 10:30	<u>T. A. Nosova</u> and Yu. M. Laevsky	Numerical Simulation of Filtration Gas Combustion
10:30 – 11:00	<u>L. Acampora</u> , G. Nigro, L. Sequino, G. Continillo and B. M. Vaglieco	Numerical Model of Spray Combustion in a Single Cylinder Diesel Engine
11:00 – 11:30	Coffee Break	



ICCMSE 2017
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21-25 April 2017

23 April 2017 SESSION: General Session I CHAIR: Zacharoula Kalogiratou (ROOM 5)		
09:00 – 09:30	Theodoros Monovasilis, Zacharoula Kalogiratou and T.E. Simos	Sixth order Two-Derivative Runge-Kutta methods.
09:30 - 10:00	Zacharoula Kalogiratou, Theodoros Monovasilis, and T.E. Simos	Modified Two-Derivative Runge-Kutta methods for solving oscillatory problems.

23 April 2017 SESSION 32: IV International Symposium of Computational and Mathematical Modeling of Biologic and Medicine Targets CHAIR: Dilson Silva and Celia M. Cortez (ROOM 5)		
10:00 – 10:30	Clicia Castro	Computer Model of Reverberant and Parallel Circuit Coupling.
10:30 – 11:00	Raimunda Fortes	A Model to Environmental Monitoring based on Glutathione-S-Transferase Activity and Brachial Lesions in Catfish.



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

23 April 2017 SESSION: Computational Chemistry Symposium (9) Honorary lecture, Highlight lecture CHAIRS: Kenichi L Ishikawa, Manabu Sugimoto (ROOM 1)		
10:35 – 11:25	Cleanthes A. Nicolaides	Honorary lecture (50 min) Nonstationary states and the many-electron problem
11:25 – 11:50	Kenichi L. Ishikawa	Implementation of the Time-Dependent Multiconfiguration Self-Consistent Field Methods for Atoms and Molecules in Intense Laser Fields
11:50 – 12:15	Y. Kuwahara	Chemical Analysis of Nanomaterials Studied by Tip-enhanced Raman Spectroscopy
12:15 – 12:40	Koichi Yamashita	Structural and Electronic Features of Hybrid Organic–Inorganic Halide Perovskite Clusters and Surfaces: Insights from First Principles
12:40 – 13:05	Vincent Robert	Macrocyclic Ligand-Driven Ferromagnetism Driven in Cu(II) Complexes
Lunch Break		



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

23 April 2017 SESSION: Computational Data Analysis and Numerical Methods CHAIR: Luis M. Grilo (ROOM 2)		
11:30 – 12:00	Filomena Teodoro	Approximating a retarded-advanced differential equation that models human phonation
12:00 – 12:30	Aldina Correia	Characterization of noise in different industrial workstations
12:30 – 13:00	Henrique Pinho	Comparative evaluation of low cost materials as constructed wetland filling media
13:00 – 13:30	Luis M. Grilo	Multinomial Logistic Regression in Workers' Health
Lunch Break		



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

23 April 2017 Symposium on Computational Methods in Economics and Nature Use CHAIR: Aleksandr N. Medvedev (ROOM 3)		
11:30 – 11:50	Olga Zvereva	Educational Network Comparative Analysis of Small Groups: short- and long-term communications
11:50 – 12:10	Olga Zvereva	Social Capital Calculations in Economic Systems: Experimental Study
12:10 – 12:30	Aleksandr Medvedev	Possibilities of Fractal Analysis of the Competitive Dynamics: Approaches and Procedures
12:30 – 12:50	Dmitry Zavalishin	Dynamic Approach to Transportation Planning under Uncertainty
Lunch Break		



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

23 April 2017 2th Symposium on Computational Combustion CHAIRS: Lucia Russo and Gaetano Continillo (ROOM 4)		
11:30 – 12:00	<u>M. Lubrano</u> <u>Lavadera, G.</u> Sorrentino, P. Sabia, M. de Joannon, R. Ragucci	Thermo kinetic instabilities in model reactor. Examples in experimental tests.
12:00 – 12:30	F. Giannino, <u>L. Russo</u> , D. Ascoli, A. Migliozzi, K. Siettos	Cellular Automata Simulation of forest fire behavior on italian landscape: the case of Sardinia
12:30 – 13:00	<u>F. Giannino</u> , D. Ascoli, M. Sirignano, A. d'Anna, S. Mazzoleni, L. Russo and F. Rego	A combustion model of vegetation burning in "Tiger" fire propagation tool
13:00 – 13:30	<u>S. Cuomo</u> , F. Giannino, S. Leveque, G. Severino and G. Toraldo	Some remarks on the numerical solution of parabolic partial differential equations
Lunch Break		



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

23 April 2017 SESSION 32: IV International Symposium of Computational and Mathematical Modeling of Biologic and Medicine Targets CHAIR: Dilson Silva and Celia M. Cortez (ROOM 5)		
11:30 – 12:00	Dilson Silva	Process Modeling of a HLA Research Lab.
12:00 – 12:30	Rafaela Brum	A Whole-Cell Simulator in GNU Octave.
12:30 – 13:00	Celia Cortez	Verifying the Competition between Haloperidol and Biperiden in Albumin through a Model based on Spectrofluorimetry.
13:00 – 13:30	Debora Batista	Micronuclei and Erythrocytic Abnormalities Frequencies of Frechwater Fishes: Establishing a Baseline for Health Status.
Lunch Break		



ICCMSE 2017

The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

Change of Schedule

23 April 2017 SESSION: Computational Chemistry Symposium (10) Light-matter interaction (1) CHAIRS: Reika Kanya, Hirokazu Hasegawa (ROOM 1)		
14:00 – 14:25	Noboru Watanabe	Angle-resolved EELS studies on vibronic coupling effects and electron-impact induced ionization dynamics
14:25 – 14:50	Valera Veryazov	Multiconfigurational chemistry: from Cr ₂ to (C ₆₀) ₂
14:50 – 15:15	Hirokazu Hasegawa	Enhancement of field-free molecular orientation of OCS by intense laser fields
15:15 – 15:40	Reika Kanya	Femtosecond gas electron diffraction by THz-wave assisted electron scattering: Numerical simulations of time-resolved electron diffraction patterns
15:40 – 16:05	Hiroshi Iwayama	State-specific dissociation dynamics of core-excited small molecules
Coffee Break		



ICCMSE 2017

**The Met Hotel, Thessaloniki, Greece,
21-25 April 2017**

23 April 2017

**SESSION: Computational Chemistry Symposium (11)
Organics (1) & Molecular chirality from a classical
and quantum point of view (1)**

**CHAIRS: Elena Besley/Federico Palazzetti, Andrea Lombardi
(ROOM 2)**

14:00 – 14:25	Hiroshi Ikeda	Amorphous Solid Simulation and Trial Fabrication of the Organic Field-Effect Transistor of Tetrathienonaphthalenes Prepared by Using Microflow Photochemical Reactions
14:25 – 14:50	Atsushi Shishido	Molecular Alignment Control for Photonic and Mechanical Applications
14:50 – 15:15	M. Besora	Computational Study of the Competitive Mechanisms in the Aromatic C-H Bond Functionalization Mediated by Coinage-Metal Catalysts
15:15 – 15:40	Yutaka Ie	Non-fullerene Acceptors for Application to Organic Photovoltaics: Structures- Thin-film Properties- Photovoltaic Characteristics Relationship
15:40 – 16:05	Federico Palazzetti	Molecular alignment and orientation in the stereodynamical selection of chirality.
16:05 – 16:30	Andrea Lombardi	Chirality in Molecular Collision Dynamics

Coffee Break



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

23 April 2017 Symposium on Computational Methods in Economics and Nature Use CHAIR: Aleksandr N. Medvedev and Marina A. Medvedeva (ROOM 3)		
15:00 – 15:30	Aleksandr Medvedev	Possibilities of fractal analysis of the competitive dynamics: approaches and procedures
15:30 – 16:00	Dmitry Zavalishin	Dynamic Approach to Transportation Planning under Uncertainty
16:00 – 16:30	Aleksandr Medvedev	Mathematical model of blasting schemes management in mining operations in presence of random disturbances
16:30 – 17:00	Valentin Kormyshev	On the Pontryagin Maximum Principle for Systems with Delays. Economic Applications
17:00 – 17:30	Coffee Break	



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

23 April 2017 2th Symposium on Computational Combustion CHAIRs: Lucia Russo and Gaetano Continillo (ROOM 4)		
15:00 – 15:30	K. Bizon, <u>G. Continillo</u> and L. Russo	On the application of POD on the study of flames
15:30 – 16:00	<u>L. Russo</u> , K. Spiliotis, F. Giannino, K. Siettos, S. Mazzoleni	Mapping regions with different dynamics in a forest/grassland model in presence of fire
16:00 – 16:30	R. Campagna, M. Brancaccio, S. Cuomo, S. Mazzoleni, L. Russo, K. Siettos and <u>F. Giannino</u>	Fire perturbation in vegetation Turing patterns
16:30 – 17:00	L. Acampora, <u>F. S. Marra</u>	Numerical Strategies for Detection of Bifurcation Points in the Parametric Continuation of Model Reactors with Detailed Chemical Mechanisms
17:00 – 17:30	Coffee Break	
Poster	M. de Joannon, G. Skevis	SMARTCATs: smart energy carrier numerical challenges for innovative systems



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

23 April 2017 SESSION 32: IV International Symposium of Computational and Mathematical Modeling of Biologic and Medicine Targets CHAIR: Dilson Silva and Celia M. Cortez (ROOM 5)		
15:30 – 16:00	Audalio Torres	Fourier Shape Descriptors in Fish Preliminary Results with Prochilodus.
16:00 – 16:30	Carolina Grassini	A Model to Estimating the Relative Position of Site for Ligands in Serum Albumins.
16:30 – 17:00	Eleuza Tenório	Antimicrobial Activity of Honey of Africanized Bee (Apis mellifera) and Stingless Bee, Tiuba (Melipona fasciculata) Against Strains of Echerichia coli, Pseudomona aeruginosa and staphylococcus aureus.
17:00 – 17:30	Coffee Break	



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

23 April 2017 SESSION: Computational Chemistry Symposium (12) Revealing mysteries of particle physics by quantum structure computation *With Cooperation of Kyoto University SPIRITS CHAIRS: Masato Senami, Koji Tsumura (ROOM 1)		
16:50 – 17:15	Masato Senami	Description of electron spin based on quantum field theory: electron electric dipole moment and chirality of a molecule and electrons.
17:15 – 17:40	Koji Tsumura	Towards Neutrino Mass Spectroscopy
17:40 – 18:05	Shigeki Matsumoto	Sommerfeld Effect on Cosmic Dark Matter
18:05 – 18:30	Akinori Fukushima	Local dielectric properties of metal oxides
18:30 – 18:55	Masahiro Fukuda	The non-equilibrium Green's function calculation based on a divide-conquer approach
18:55 – 19:20	M. Yamanaka	Search for charged lepton flavor violation using a muonic atom
Dinner		



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

Change of Schedule

23 April 2017 SESSION: Computational Chemistry Symposium (13) Molecular chirality from a classical and quantum point of view (2) & Organics CHAIRS: Federico Palazzetti, Andrea Lombardi (ROOM 2)		
16:50 – 17:15	Vincenzo Aquilanti	The astrochemical observatory: experimental and computational search of the chiral molecule propylene oxide as a case study
17:15 – 17:40	Toshio Kasai	Role of Cooperative Network Interaction in Transition Region of Roaming Reactions: Non-Equilibrium Steady State vs. Thermal Equilibrium Reaction Scheme
17:40 – 18:05	King-Chuen Lin	Angular Distribution of Bromine Atomic Photofragment in Oriented 2-Bromobutane Via Hexapole State Selector
18:05 – 18:30	Cecilia Coletti	Perspectives in the study of chiral recognition through IRMPD spectroscopy: Experiments and Computations.
18:30 – 18:55	Shigenori Fujikawa	Precise molecular separation by designed nanomembrane
Dinner		



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

23 April 2017 Symposium on Computational Methods in Economics and Nature Use CHAIR: Aleksandr N. Medvedev and Marina A. Medvedeva (ROOM 3)		
17:30 – 18:00	Valentin Kormyshev	Ordinary Multiplication of Distributions. Application to Control of Economic Processes
18:00 – 18:30	Alexandr A. Tarasyev	Optimization of Educational Paths for Higher Education
18:30 – 19:00	Alexandr A. Tarasyev	Value Function in Economic Growth Model
19:00 – 19:30	Valentin Kormyshev	Differential Games in Economic Systems with Delays
19:30 – 20:00	Valentin Kormyshev	On Control of Systems Delays in Economics

23 April 2017 SESSION: General Session I CHAIR: Constantinos Siettos (ROOM 5)		
18:15 – 18:45	Ioannis Gallos and Constantinos Siettos	Classification of fMRI Resting-State Maps using Machine Learning Techniques: a Comparative Study



ICCMSE 2017

**The Met Hotel, Thessaloniki, Greece,
21-25 April 2017**

23 April 2017

**SESSION: Application of New Physical Theories, Methods
and Technics in Biology and Medicine**

**CHAIR: AtanasTodorov Atanasov
(ROOM 4)**

17:30 – 18:00	Atanas T. Atanasov	Is applicable thermodynamics of negative temperature for living organisms?
18:00 – 18:30	Atanas T. Atanasov	Thermodynamics of the living organisms. Allometric relationships between total metabolic energy, chemical energy and body temperature in Mammals
18:30 – 19:00	BoyanaParvanova, BilyanaTacheva, Miroslav Karabaliev, Ivan Ivanov	Thermal dielectroscopy – a new method for studying the membrane skeleton of human erythrocytes
19:00 – 19:30	Bilyana Tacheva, BoyanaParvanova, Ivan Ivanov, Miroslav Karabaliev	Impedance dispersion analyses of drug-membrane interaction

23 April 2017

**SESSION 32: IV International Symposium of
Computational and Mathematical Modeling of Biologic
and Medicine Targets**

**CHAIR: Dilson Silva and Celia M. Cortez
(ROOM 5)**

17:30 – 18:00	Celia Cortez	A Model based on Spectrofluorimetry to Study the Interaction between Glyphosate and Serum albumin of Salminus brasiliensis.
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END OF THE 2ND DAY



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

24 April 2017 SESSION: Computational Chemistry Symposium (14) Highlight lecture CHAIR: Matthias Ernzerhof (ROOM 1)		
8:30 – 8:55	Paul Geerlings	The Linear Response Function of Conceptual Density Functional Theory: from Mathematical Properties to Applications in Single Molecule Electronics
8:55 – 9:20	Jan M. L. Martin	Noncovalent Interactions: Rigorous Answers Through Explicitly Correlated Ab Initio Methods And Assessment Of More Approximate Methods
9:20 – 9:45	Takanori Fukushima	Controlled Assembly of Functional Molecules Using Supramolecular Scaffolds
9:45 – 10:10	Elena Besley	When do clusters of the same charge attract?
10:10 – 10:35	A.L. Tchougréeff	Περὶ τοῦ στοιχείου τοῦ υδατος or Deductive Molecular Mechanics of Crystalline Polymorphs of Water
Coffee Break		



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

Change of Schedule

24 April 2017 SESSION: Computational Chemistry Symposium (15) Highlight lecture, Keynote Lecture CHAIR: Hiroshi Nakanishi (ROOM 1)		
10:45 – 11:10	Dennis R. Salahub	Multiscale Modeling of Chemical Reactions in Complex Environments
11:10 – 11:35	Hikaru Kobayashi	Hydrogen generation by the reaction of Si nanopowder with water
11:35 – 12:00	Karin Larsson	A combinatorial effect of substrate and surface terminating species on phase pure growth of c-BN
12:00 – 12:25	Pavel Hobza	Quantum mechanical scoring function: most accurate and efficient tool for computational drug design



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

24 April 2017 SESSION: General Session III CHAIR: Ivan Valent (ROOM 3)		
09:00 – 09:30	Ivan Valent	Kinetics of the Electric Double Layer Formation Modelled by the Finite Difference Method
09:30 – 10:00	Dongjie Chen, Wensheng Zhang and Yang Yang	High-speed Railway Real-time Localization Auxiliary Method based on Deep Neural Network
10:00 – 10:30	Linna Liu and Feiqi Deng	Stability of Euler-Maruyama Numerical Schemes for Time Varying Delayed Stochastic Hopfield Neural Networks
10:30 – 11:00	Linda Smail	Variable Elimination Algorithm: An Updated Version



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

24 April 2017

13:30 - 18:30

Central Excursion

24 April 2017

20:30 - 24:00

Central Dinner

END OF THE 3RD DAY



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

25 April 2017 SESSION: Computational Chemistry Symposium (16) Theory (2), Light-matter interaction (2) CHAIR: Noboru Watanabe (ROOM 1)		
8:30 – 8:55	Nobuhiko Sarukura	TBA
8:55 – 9:20	Yasushi Kino	Nuclear reaction in atomic collision under a screening effect from negatively charged massive particle
9:20 – 9:45	Heide Ibrahim	Imaging and controlling proton motion in molecules
9:45 – 10:10	Benoit Mignolet	Modeling the electron-nuclear dynamics induced by short laser pulses in molecules with the Ab-Initio Multiple Spawning (XFAIMS) method
10:10 – 10:35	Jan M. L. Martin	Toward a W4-F12 approach: Can explicitly correlated and orbital-based ab initio CCSD(T) limits be reconciled?
Coffee Break		



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

25 April 2017 SESSION: Computational Chemistry Symposium (17) Organics (2) CHAIR: Nathalie Guihéry (ROOM 2)		
8:30 – 8:55	Taye B. Demissie	How does a single electron affects NMR?
8:55 – 9:20	Keishiro Tahara	Fabrication of Covalent- and Hydrogen-Bonded Assemblies of Biferrocenium Diboronic Acid and Their Charge Transfer Properties
9:20 – 9:45	Haruyuki Okamura	Synthesis of I-line or G-line Sensitive Photoacid Generators and Their Application to Photosensitive Materials
9:45 – 10:10	Azusa Muraoka	Solvent effects on the helical reaction path of o-phenylene derivatives
Coffee Break		

25 April 2017 SESSION: General Session IV CHAIR: George D. Verros (ROOM 3)		
09:00 – 09:30	George D. Verros and Maria Papachristou	Towards to the Development of a Detailed Computational Chemical Geothermometer
09:30 – 10:00	M. Perl P and M. Steiner	Numerical Evaluation of an Internally Cracked Autofrettaged Spherical Pressure Vessel
10:00 – 10:30	D. V. Alexandrov and P. K. Galenko	Dendritic Growth in an Inclined Viscous Flow. Part 1. Hydrodynamic Solutions



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

25 April 2017 SESSION: General Session V CHAIR: Liana Kovaleva (ROOM 4)		
09:00 – 09:30	Nicola Grillanda, Fabio Manconi, Flavio Stochino, Antonio Cazzani, Francesco Bondi, Andrea Chiozzi, Antonio Tralli	On the Analysis of the Stellar Vault of Santa Maria del Monte in Cagliari
09:30 – 10:00	Alfred Davletbaev, Liana Kovaleva, Victor Kireev, Aleksey Zainullin, Artem Myasnikov	Solvent Injection and Radio-Frequency Electromagnetic Radiation in the Fractured Well: Numerical Study
10:00 – 10:30	Victor Kireev, Liana Kovaleva, Andrey Isakov and Sofya Alimbekova	Numerical Investigation of the Influence of Electromagnetic Treatment on Calcium Carbonate Scaling Rate in Non-Isothermal Pipe Flow
10:30 – 11:00	O.A. Dobrozhan, P.S. Danilchenko, D.I. Kurbatov and A.S. Opanasyuk	Optical and recombination losses in the solar cells with n-ITO(ZnO)/n-CdS(ZnS, ZnSe)/p-Cu₂ZnSnS₄ structures
11:00 – 11:30	Coffee Break	



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

Change of Schedule

25 April 2017 SESSION: Computational Chemistry Symposium (18) Dynamics (2) CHAIRS: Titus S. van Erp, Gabriel Hanna (ROOM 1)		
10:45 – 11:10	Titus S. van Erp	Concerted and stepwise autoionization of water
11:10 – 11:35	Takatsugu Hirokawa	Ligand binding site analysis with protein flexibility for ligand docking, lead optimization and virtual screening
11:35 – 12:00	Hisashi Okumura	All-Atom Molecular Dynamics Simulations to Reveal Dynamical Ordering of Amyloid Fibril
12:00 – 12:20 (20 min)	Paul Bauer	Computational models for the study of enzyme evolution and promiscuity
Lunch Break		



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

Change of Schedule

25 April 2017 SESSION: Computational Chemistry Symposium (19) Materials (2) CHAIR: Wilson Agerico Diño (ROOM 2)		
10:45 – 11:10	Daisuke Kan	Interface engineering of metal-oxygen bonds as a new route for exploring functional properties of transition metal oxides
11:10 – 11:35	Teppei Ogura	Computational Analysis for The Reaction Mechanism of Steam Methane Reforming Considering Surface Morphology of Nickel Catalysts
11:35 – 12:00	Masataka Kubo	Novel Specialized Polymeric Materials from Experimental Chemists: Emitting Polymer/Silica Hybrids and Network Polymers with Movable Cross-Linking Points
12:00 – 12:20 (20 min)	A. S. Hutama	Density-Functional Tight-Binding Repulsive Potentials for Zr – Zr Interactions in Bulk Zirconium
Lunch Break		



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

25 April 2017 SESSION: General Session VI CHAIR: D. V. Alexandrov (ROOM 3)		
11:30 – 12:00	D. V. Alexandrov and P. K. Galenko	Dendritic Growth in an Inclined Viscous Flow.Part 2. Numerical Examples
12:00 – 12:30	D. V. Alexandrov, I. V. Alexandrova, A. A. Ivanov	The Role of Nonlinear Mass Transport on Directional Crystallization with a Mushy Layer
12:30 – 13:00	Ilya Starodumov, Peter Galenko, Nikolai Kropotin and Dmitri V. Alexandrov	Influence of Initial Seed Distribution on The Pattern Formation of The Phase Field Crystals
13:00 – 13:30	T. Kireev and G. Bulgakova	Multiphase Flow Simulation in the Finite Conductivity Fracture for the Full-field Modeling

25 April 2017 SESSION: General Session VII CHAIR: Valeriy Perminov (ROOM 4)		
11:30 – 12:00	LI Zheng-guo, WANG Genping, SUN Xiaoli	Harmonic Detection of power system Based on Hamming Windowed FFT and Wavelet packet Transform
12:00 – 12:30	Valeriy Perminov and Elina Soprunenkoe	Mathematical Modeling of Three-Dimensional Crown Wildfire Initiation
12:30 – 13:00	Tomasz Jastrzab and Agata Buchcik	A Parallel Algorithm for Finding the Shortest Exit Paths in Mines
13:00 – 13:30	Diana-Elena Tudorache	A Numerical Investigation of Reactive Jet Interaction in a Steam Methane Reformer



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

25 April 2017 SESSION: Computational Chemistry Symposium (20) Oral presentation, Short oral presentation* CHAIR: Hisashi Okumura (ROOM 2) *10 min without question		
13:30 – 13:50 (20 min)	Yuki Oba	Path integral simulation on muoniated acetone radical
13:50 – 14:00 (10 min)	Yosuke Sumiya	Conformational Entropy of Unimolecular Reactions Studied by a New Kinetic Approach
14:00 – 14:10 (10 min)	Chihiro Tokizaki	Theoretical analyses of the time-resolved nuclear dynamics of the transition state for the cyclooctatetraene unimolecular reaction
14:10 – 14:20 (10 min)	Yusuke Seki	A simulation study of photoexcited Ag ejection from low-temperature helium clusters by ring-polymer molecular dynamics
14:20 – 14:30 (10 min)	Evgheni Jucov	Structural and Computational Studies of the New Polymorph of Tetracene-TCNQ
14:30 – 14:40 (10 min)	Gil R. Gallegos	Computational Plasmonics and Hybrid Ensemble-Deep Neural Network Machine Learning Methods Utilized for Predictive Response of a Randomly Distributed Nanostar Substrate with Applications in Bio-Sensor Design



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

25 April 2017 SESSION: 11 Advances In Financial Systems Modelling and Control CHAIR: G. Rigatos and P. Siano (ROOM 1)		
15:00 – 15:30	G. Rigatos, P. Siano, V. Loia, A. Tommasett and O. Troisi	A nonlinear optimal control approach for chaotic finance dynamics
15:30 – 16:00	G. Rigatos, P. Siano, T. Ghosh and D. Sarno	Stabilization of business cycles of finance agents using nonlinear optimal control
16:00 – 16:30	G. Rigatos, P. Siano, V. Loia, A. Tommasetti and O. Troisi	Flatness-based adaptive fuzzy control of chaotic finance dynamics
16:30 – 17:00	G. Rigatos, P. Siano, T. Ghosh, K. Busawon and R. Binns	Flatness-based control and Kalman Filtering for a continuous-time macroeconomic model
Poster	Tana Sebechlebska and Ivan Valent	Effect of Concentration, Ionic Strength and Charge Number on Electrodifusion in a Simple Membrane Channel



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

25 April 2017 SESSION: General Session VIII CHAIR: S.I. Solodushkin (ROOM 3)		
15:00 – 15:30	Iumanova I. F., Solodushkin S. I. and Sagoyan A. A.	One Modification of Steffensen's Method for Operator Equations and Its Applications
15:30 – 16:00	Shen Weidong, Tian Baolin	A Multimaterial Arbitrary Lagrangian-Eulerian Method for Rayleigh-Taylor Instability
16:00 – 16:30	Juri Selvåg, Tatiana Kuznetsova and Bjørn Kvamme	Molecular Dynamics Study of N- Formyl Morpholine Surfactant in CO₂/H₂O/Oil Interfacial System



ICCMSE 2017
The Met Hotel, Thessaloniki, Greece,
21-25 April 2017

25 April 2017 SESSION: 11 Advances in Financial Systems Modelling and Control CHAIR: G. Rigatos and P.Siano (ROOM 1)		
17:00 – 17:30	G. Rigatos, P. Siano and D. Sarno	A boundary PDE feedback control approach for the stabilization of mortgage price dynamics
17:30 – 18:00	G. Rigatos, P. Siano, T. Ghosh and D. Sarno	A nonlinear optimal control approach to stabilization of a macroeconomic development model
18:00 – 18:30	G. Rigatos, P. Siano, V. Loia, S. Ademi and T. Ghosh	Nonlinear optimal control for the synchronization of chaotic and hyperchaotic finance systems

END OF THE 4TH DAY
END OF THE CONFERENCE