



ICCMSE 2018
The Met Hotel, Thessaloniki, Greece,
14-18 March 2018

15 March 2018 SESSION: Computational Chemistry Symposium (1) Highlight I, Artificial Photosynthesis and Catalyst (APC) I CHAIR: Tokuei Sako, Taku Onishi (ROOM 1)		
8:20 – 8:30	Opening Ceremony Theodore Simos (Chairman of ICCMSE 2018)	
8:30 – 8:55	<i>Taku Onishi</i>	A Theoretical Study of Hydrogen Anion Transport in BaTiO₃ Perovskite
8:55 – 9:20	<i>Kazunari Domen</i>	Particulate photocatalysts for water splitting using solar energy
9:20 – 9:45	<i>Kyoko Nozaki</i>	Mechanistic Studies on The Pd-Catalyzed Copolymerization of Olefins with Polar Monomers
9:45 – 10:10	<i>Osamu Ishitani</i>	Photochemical and electrochemical reduction of low concentration of CO₂
10:10 – 10:30	Group Photo	
Coffee Break (The coffee break will be available between 10:30 - 11:30)		



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15 March 2018 SESSION: Computational Chemistry Symposium (2) Highlight II CHAIR: Andrei L. Tchougréeff (ROOM 1)		
11:00 – 11:25	<i>Tamio Oguchi</i>	Crystal Structure Search for Materials Discovery
11:25 – 11:50	<i>Dmitri Sokolovski</i>	SIMULATIONS OF CHEMICAL REACTIONS: SOFTWARE FOR ANALYSING RESONANCE EFFECTS
11:50 – 12:15	<i>Jan M. L. Martin</i>	Do Conventional And Explicitly Correlated Coupled Cluster Theory Converge To The Same Limits? Computational Evidence And Perturbation Theoretical Analysis
12:15 – 12:40	<i>Elena V. Orlenko</i>	Spin-Exchange and Spin- Orbit Interaction in Fullerenes
Lunch Break		



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15 March 2018 SESSION: 2nd Symposium on Computational Simulation and Experimental Analysis of Hygrothermal Phenomena in Building Envelopes CHAIR: Jan Fořt (ROOM 2)		
09:00 – 09:20	<i>Eva Vejmelková, Jan Fořt, Aneta Junková, Monika Čáchová, Pavla Rovnaníková and <u>Robert Černý</u></i>	Thermal and hygric properties of alkali activated aluminosilicates
09:20 – 9:40	<i><u>Miloš Jerman,</u> Vratislav Tydlitát and Robert Černý</i>	Early age calorimetric investigations of geopolymers
9:40 – 10:00	<i><u>Václav Kočí,</u> Jiří Maděra and Robert Černý</i>	Computational Analysis of Thermal Processes at Early- Age Hydration of Lime-based Binders
10:00 – 10:20	<i>Michaela Petříková, Magdaléna Doleželová, Jaroslav Dušek, <u>Lukáš Fiala,</u> and Robert Černý</i>	Heat, Water and Water Vapour Transport and Storage Properties of Alkali-Activated Aluminosilicates
10:20 – 10:40	<i>Lukáš Fiala, <u>Jiří Maděra,</u> and Robert Černý</i>	Computational Simulation of Transport Phenomena in Self- Heating Aluminosilicate Composites
10:40 – 11:00	<i><u>Jiří Zach,</u> Jitka Peterková, Vítězslav Novák</i>	Study of heat transfer process in structure of fiber based materials under low pressure



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<p>15 March 2018</p> <p>SESSION: 2nd Symposium on Computational Simulation and Experimental Analysis of Hygrothermal Phenomena in Building Envelopes</p> <p>CHAIR: Václav Kočí (ROOM 2)</p>		
<p>11:30 – 11:50</p>	<p><u>Jan Fořt</u> and <u>Robert Černý</u></p>	<p>Environmental assessment of mineral wool manufacturing</p>
<p>11:50 – 12:10</p>	<p><u>Magdaléna Doleželová, Jiří Maděra, Alena Vimmrová</u></p>	<p>Experimental determination of mechanical parameters for damage modelling of gypsum- based composites</p>
<p>12:10 – 12:30</p>	<p><u>Lenka Scheinherrová, Magdaléna Doleželová, Alena Vimmrová</u></p>	<p>Optimizing Database Architecture for the Thermal Analysis Results of Building Materials</p>
<p>12:30 – 12:50</p>	<p><u>Jan Kočí, Jiří Maděra and Robert Černý</u></p>	<p>Formulation of Hygrothermal Model for Description of Ice- forming Process in Porous Building Materials</p>
<p>12:50 – 13:10</p>	<p><u>Jan Kočí, Jiří Maděra, Juliana Maria da Silva, Zuzana Hlaváčová and Robert Černý</u></p>	<p>Hygrothermal Model for Description of Ice-forming Process in Porous Building Materials: Sensitivity Analysis of Input Material Parameters</p>



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SESSION: Computational Chemistry Symposium (3)		
Chemical physics on chirality and related aspects I		
CHAIR: Andrea Lombardi		
(ROOM 1)		
13:30 – 13:55	<i>Federico Palazzetti</i>	Alignment and orientation in the stereodirected photodissociation dynamics of chiral molecules.
13:55 – 14:20	<i>Cecilia Coletti</i>	Stereodynamics effects on reactive and inelastic scattering highlighted by the inclusion of long range potential: the OH+H₂ case study
14:20 – 14:45	<i>Concetta Caglioti</i>	Configurational plots of four-center systems and characterization of chirality changing processes



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<p style="text-align: center;">15 March 2018 SESSION: Computational Chemistry Symposium (4)(5) Chemical physics on chirality and related aspects II CHAIR: Federico Palazzetti Current topics related to quantum physics -particle physics, cosmology, and fundamental theory- I CHAIR: Shigeki Matsumoto (ROOM 1)</p>		
15:20 – 15:45	<i>Andrea Lombardi</i>	Collisions of chiral molecules: theoretical aspects and experiments
15:45 – 16:10	<i>Inbal Tuvi-Arad</i>	Measuring symmetry and Chirality – New Algorithms for Generic Structural Analysis
16:10 – 16:35	<i>Masato Senami</i>	Asymmetry of Electron Chirality between Enantiomeric Pair Molecules and the Origin of Homochirality in Nature
16:35 – 17:00	<i>Masahiro Kawasaki</i>	Formation of primordial black holes in multi-field inflation models
<p style="text-align: center;">Coffee Break (The coffee break will be available between 16:30 - 17:30)</p>		



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15 March 2018 SESSION: Computational Chemistry Symposium (6) Current topics related to quantum physics Current topics related to quantum physics -particle physics, cosmology, and fundamental theory- II, Oral Presentation CHAIR: Masato Senami (ROOM 1)		
17:30 – 17:55	<i>Shigeki Matsumoto</i>	Chemistry of Dark Matter
17:55 – 18:20	<i>Shigenori Seki</i>	Entanglement Entropy of Scattering Particles
18:20 – 18:40 (20 min)	<i>Hajime Fukuda</i>	Quantum Mechanical Effect on the Direct Detection of Ultralight Dark Matter
18:40 – 18:50 (10 min)	<i>Toshiki Takahashi</i>	Effective electric field for measurement of electron electric dipole moment and local spin dynamics based on quantum field theory



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15 March 2018 SESSION: Computational Chemistry Symposium (7) Biology I CHAIR: Noam Agmon (ROOM 2)		
13:30 – 13:55	<i>Yoshie Harada</i>	Development of a new fluorescence imaging technique using nitrogen vacancy centers in diamond.
13:55 – 14:20	<i>Takefumi Yamashita</i>	Structural effects on the antigen-antibody interaction: Insight from molecular dynamics simulations of biopolymers



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15 March 2018 SESSION: Computational Chemistry Symposium (8) Artificial Photosynthesis and Catalyst (APC) II CHAIR: Nathalie Guihéry (ROOM 2)		
15:20 – 15:45	<i>Hiroshi Nakanishi</i>	DFT-Guided Design of Catalysts for Methane Activation
15:45 – 16:10	<i>Yoong-Kee Choe</i>	Catalytic Conversion of Ethanol to Butadiene: A DFT Study of the Complex Reaction Mechanism
16:10 – 16:35	<i>Ignacio Funes-Ardoiz</i>	Computational Characterization on the Active Role of the Oxidant in Oxidative Coupling Reactions
16:35 – 17:00	<i>Joe Otsuki</i>	Photo/electronic processes in multimetal coordination compounds
Coffee Break (The coffee break will be available between 16:30 - 17:30)		



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15 March 2018		
SESSION: Computational Chemistry Symposium (9)		
Materials I		
CHAIR: Toshinori Okura, Pavel A. Korzhavyi		
(ROOM 2)		
17:30 – 17:55	<i>Toshinori Okura</i>	Development of Na⁺-Fast Ionic Conducting Narpzio Glass-Ceramics
17:55 – 18:20	<i>Pavel A. Korzhavyi</i>	Exploring configurational degrees of freedom in disordered solids
18:20 – 18:45	<i>Simone Taioli</i>	The chemistry and physics of carbon from first-principles, multiscale simulations, and experiments
18:45 – 19:10	<i>Takeshi Nakanishi</i>	Effective-mass theory of inter-layer interaction in bi-layer graphene and collapsed carbon nanotubes



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15 March 2018 ICCMSE 2018 HIGHLIGHTED INVITED SPEAKER CHAIR: Taku Onishi (ROOM 1)		
20:30 – 21:20	<i>Paul Mezey</i>	Exploiting the Freedom of Abstraction and Virtual Reality in Molecular Modelling: Some General Modelling Principles with Analogies of the Complex Plane

15 March 2018 21:20 – 23:00 WELCOME DRINK
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15 March 2018 Poster Session of Computational Chemistry Symposium 21:30 – 22:30	
<i>Shogo Kunieda</i>	Surface Structure Chemical Transfer (SSCT) Method for Fabrication of Low Reflectance and High Carrier Lifetime Textured Multi-Crystalline Silicon
<i>Toshiki Takahashi</i>	Effective electric field for measurement of electron electric dipole moment and local spin dynamics based on quantum field theory
<i>Hajime Fukuda</i>	Quantum Mechanical Effect on the Direct Detection of Ultralight Dark Matter
<i>Kento Suzuki</i>	Real-time nonadiabatic ionization dynamics of low-temperature helium clusters using ring-polymer MD method
<i>Eiki Ozama</i>	Path Integral Molecular Dynamics study on structures of Ac ³⁺ -doped helium clusters
<i>Serguei Feskov</i>	The time-dependent j-flux method for stochastic simulations of multistage bimolecular photoinduced electron transfer within the extended integral encounter theory
<i>Serguei Feskov</i>	FLUT: a numerical code for simulations of multistage bimolecular photoinduced electron transfer reactions in viscous solutions
<i>Kohei Sasaki</i>	Influence of the point-charge modeling on the structure of mixtures of epoxy resin and amine-curing agent observed in molecular dynamics simulations
<i>Hajime Suzuki</i>	Z-scheme water splitting using tungstic acids as oxygen-evolving photocatalysts under visible light

END OF THE 1ST DAY



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16 March 2018 SESSION: Computational Chemistry Symposium (10) Highlight III, Light-Matter Interaction (LM) I CHAIR: Taku Onishi, Tokuei Sako (ROOM 1)		
8:30 – 8:55	<i>Tokuei Sako</i>	Light-matter interaction in ICCMSE 2018
8:55 – 9:20	<i>Nils Schopohl</i>	On the Theory of Light Propagation in Crystalline Dielectrics
9:20 – 9:45	<i>Andrei L. Tchougréeff</i>	Spin-Liquids: A Lost Tribe of Solid-State Quantum Chemistry.
9:45 – 10:10	<i>Aurora Clark</i>	Advances in Graph Theory Methods for Characterizing and Driving Condensed Phase Organization, Dynamics, and Reactivity
10:10 – 10:35	<i>Berta Fernández</i>	The Helical Sense of Poly(phenylacetylene)s from Electron Circular Dichroism Spectra: A Computational Evaluation
Coffee Break (The coffee break will be available between 10:30 - 11:30)		



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<p>16 March 2018</p> <p>MS15: Existing and New Structures in Seismic Prone Areas: Advanced Numerical Modelling and Experimentation</p> <p>CHAIR: F. Clementi, G. Milani, A. Formisano</p> <p>(ROOM 2)</p>		
09:00 – 09:25	<u><i>Ribilotta E., Clementi F., Pellegrino M., Poiani M., Gazzani V., Santilli G., Lenci S.</i></u>	<p>Monitoring cultural heritage buildings: The San Ciriaco bell-tower in Ancona, Italy</p>
09:25 – 09:50	<u><i>Habieb B.A., Milani G., Tavio, Milani F.</i></u>	<p>An Abaqus UEL for the structural implementation of low-cost rubber seismic isolators in masonry buildings</p>
09:50 – 10:15	<u><i>Fonti R.</i></u>	<p>The Justice Palace of Messina. Between innovation and tradition.</p>
10:15 – 10:40	<u><i>Clementi F., Milani G., Gazzani V., Poiani M., Cocchi, G., Lenci S.</i></u>	<p>The Non-Smooth Contact Dynamics method for the analysis of ancient masonry towers</p>
10:40 – 11:05	<u><i>Formisano A., Fonti R.</i></u>	<p>The role of massive vaults and buttresses in masonry building aggregates: a case study</p>
11:00 – 11:30	<p>Coffee Break (The coffee breaks will be available between 10:30 - 11:30)</p>	



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16 March 2018 SESSION: Modern Information Technology as an Instrument Used in Sport, Tourism and Recreation to Build a Healthy Society CHAIR: Mirosława Szark-Eckardt and Hanna Żukowska (ROOM 3)		
09:00 – 09:30	<i>Hanna Żukowska, Michalina Kuska</i>	<i>The use of modern information technologies by seniors citizens regarding health</i>
09:30 – 10:00	<i>Iwona Józefowicz</i>	<i>Geocaching in Poland. Spatial aspect</i>
10:00 – 10:30	<i>Mirosława Szark-Eckardt</i>	<i>Mobile applications as a tool conditioning health of young generation</i>
10:30 – 11:00	<i>Jolanta Grażyna Zuzda, Piotr Borkowski, Robert Latosiewicz</i>	<i>Thermographic Imaging as a Computer Method of Training Efficiency Measurement in Preparation for Tourist Activity</i>
11:00 – 11:30	Coffee Break (The coffee breaks will be available between 10:30 - 11:30)	



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16 March 2018 SESSION: Computational Data Analysis and Numerical Methods CHAIR: Luis M. Grilo (ROOM 4)		
09:00 – 09:30	<i>Eliana Costa e Silva</i>	How Portuguese expert perceptions' on the entrepreneurial framework conditions have changed over the years?
09:30 – 10:00	<i>Ana Borges</i>	A Joint Model of Time to Breast Cancer Recurrence and CA15-3 Marker Longitudinal Progression
10:00 – 10:30	<i>Filomena Teodoro</i>	Estimating Childhood Hypertension Prevalence in Some Regions of Portugal: a Preliminary Approach
10:30 – 11:00	<i>Cristina Dias</i>	Model Validation and Vec Operators
11:00 – 11:30	Coffee Break (The coffee breaks will be available between 10:30 - 11:30)	



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16 March 2018 SESSION: Computational Chemistry Symposium (11) Highlight IV, Artificial Photosynthesis and Catalyst (APC) III CHAIR: Hiroshi Nakanishi (ROOM 1)		
11:00 – 11:25	<i>Katsuyuki Fukutani</i>	Adsorption and diffusion of hydrogen on metal-oxides surfaces
11:25 – 11:50	<i>Isao H. Inoue</i>	Artificial synapses and neurons based on an insulator-to-2D metal transition of a SrTiO₃ surface.
11:50 – 12:15	<i>Koichi Yamashita</i>	Charge Separation and Charge Carrier Trapping of Lead Iodide Perovskites
12:15 – 12:40	<i>Ryu Abe</i>	Design of Stable Mixed-Anion Semiconductors for Photocatalytic Water Splitting under Visible Light
Lunch Break		



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16 March 2018		
SESSION 20: V International Symposium of Computational and Mathematical Modeling of Biology and Medicine		
Targets		
CHAIR: Dilson Silva		
(ROOM 2)		
11:30 – 12:00	<u>Raimunda Fortes</u>	A Model to Environmental Risk Assessment Based on Biochemical and Morphological Biomarkers in catfish
12:00 – 12:30	<u>Ligia Tchaicka</u>	Micronucleus Test in <i>Centropomus undecimalis</i> (BLOCH, 1972) for the Assessment of the Water Quality of two Brazilian Estuaries
12:30 – 13:00	<u>Raimunda Fortes</u>	Models of Sexual Maturation as a Tool for the Conservation of Commercial Fish in a RAMSAR Site of Brazil
13:00 – 13:30	<u>Lais N. Alves</u>	Selection and Evaluation of the Binding of Aptamers Against NS5 Zika Virus Using Fluorescence Spectroscopy



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16 March 2018 SESSION: Modern Information Technology as an Instrument Used in Sport, Tourism and Recreation to Build a Healthy Society CHAIR: Mirosława Szark-Eckardt and Hanna Żukowska (ROOM 3)		
11:30 – 12:00	<i>Mirosława Szark-Eckardt, Jadwiga Nidzgorska-Lencewicz, Agnieszka Makosza, Hanna Żukowska</i>	<i>Usability of weather portals in sport, tourism and recreation in the opinion of young people (students).</i>
12:00 – 12:30	<i>Wioletta Lubkowska</i>	<i>Application of the computerized functional diagnosis system with the sensor Wiva® Science in the evaluation of the effectiveness of rehabilitation of patients with back pain syndrome</i>
12:30 – 13:00	<i>Wioletta Lubkowska, Michał Tarnowski, Robert Terczynski.</i>	<i>Time measurement of a 30-meter run, using the cinematographic method and photogrammetry as an example of applying modern technology in promoting physical activity</i>
13:00 – 13:30	<i>Marcin Pasek Remigiusz Drózdź</i>	<i>Modern technologies in the hotel industry as a condition of the safety of tourists</i>



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16 March 2018 SESSION: Computational Data Analysis and Numerical Methods CHAIR: Luis M. Grilo (ROOM 4)		
11:30 – 12:00	<i>Maria Varadinov</i>	A Study on Reverse Logistics for Medicines Supply in Hospital Pharmacies
12:00 – 12:30	<i>Luis M. Grilo</i>	Structural equation modelling using partial least square approach to assess workers burnout state

16 March 2018 SESSION: The First Symposium on Information, Intelligent, Education and Engineering Application CHAIR: CHIALIANG LIN (ROOM 4)		
13:00 – 13:30	<i>Yuchen Shen</i>	Comparison of Self-regulation between Students in Taiwan and Yunnan to Academic Performance Presented
13:30 – 14:00	<i>LUNGCHUAN CHIANG</i>	Design and Testing of an Instrument to Measure Cultural Competence among College Seniors. A Preliminary Study
14:00 – 14:30	<i>CHIALIANG LIN</i>	The Efficiency Evaluated System for solar panel by Drone with Infrared Sensor



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<p>16 March 2018</p> <p>SESSION: Computational Data Analysis and Numerical Methods</p> <p>CHAIR: Luis M. Grilo</p> <p>12:30 – 13:30</p>	
<p>Title (oral presentation)</p>	
<p>Luís M. Grilo, Helena L. Grilo and Elisa Martire</p>	<p>SEM using PLS Approach to Assess Workers Burnout State</p>
<p>Title (poster)</p>	
<p>Fátima De Almeida, Eliana Costa e Silva and Aldina Correia</p>	<p>Dispersion of the Organoclay C15A Along the Screw Profile: Using TEM to Compare PP Nanocomposites Thickness</p>
<p>Lara Teixeira, Vasco Machado, A. Manuela Gonçalves, Susana Faria and Manuela Felício</p>	<p>Statistical Analysis of Health Inequalities in the Northern Region of Portugal</p>
<p>Sérgio Nunes, Vanda Sousa and Luís M. Grilo</p>	<p>Perfect Resources, Singularities and Scientific Tourism: Methodological Contributions to Valuation and Resources Institutionalization</p>
<p>Fernanda Otilia Figueiredo, Adelaide Otilia Figueiredo and Maria Ivette Gomes</p>	<p>Design of Sampling Plans for Sensory Evaluation</p>
<p>Dina M. R. Mateus, Henrique J. O. Pinho and Luís M. Grilo</p>	<p>Evaluation of the Sugar Content along the Stalk Height of Sugarcane Plants for Different Growth Conditions. Statistical Analysis.</p>
<p>M. Filomena Teodoro</p>	<p>Some Applications of Mixed Type Functional Equations</p>



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16 March 2018 SESSION: Computational Chemistry Symposium (12) Theory I CHAIR: Gabriel Hanna, Serguei Feskov (ROOM 1)		
13:55 – 14:20	<i>Shinnosuke Kawai</i>	Essential Dynamical Coordinates to Describe Quantum Mechanical Systems
14:20 – 14:45	<i>Satoshi Takahashi</i>	Beyond semiclassics for nuclear dynamics in molecules



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16 March 2018		
SESSION: Computational Chemistry Symposium (15)		
Materials II		
CHAIR: David J. Henry, Oded Hod		
(ROOM 2)		
13:30 – 13:55	<i>David J. Henry</i>	Exploring the Bonding and Reactivity Trends in Gallium Nanoclusters
13:55 – 14:20	<i>Yuki Kobayashi</i>	Hydrogen Generation from Si Nanopowder by Reaction with Neutral Water
14:20 – 14:45	<i>Oded Hod</i>	Modeling Interlayer Interactions in Layered Materials
14:45 – 15:10	<i>Yuji Kunisada</i>	Diffusion of a single atom on heteroatom-doped graphene



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16 March 2018		
SESSION: Computational Chemistry Symposium (13)		
Theory II		
CHAIR: Valera Veryazov, Sergei F. Vyboishchikov		
(ROOM 1)		
15:20 – 15:45	<i>Valera Veryazov</i>	Multiconfigurational study of Cr₂ and Cr₂⁺
15:45 – 16:10	<i>Sergei F. Vyboishchikov</i>	Exchange-Correlation Potentials and Energy Densities in Spherically Confined Atoms
16:10 – 16:35	<i>Paweł Szarek</i>	The Clear-Cut Radii of Atoms and Ions: Free and in Chemical Compounds
16:35 – 17:00	<i>Yuhki Ohtsuka</i>	Selected Configuration Interaction Method Using Sampled First-Order Corrections to Wave Functions
Coffee Break		
(The coffee break will be available between 16:30 - 17:30)		



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16 March 2018 SESSION: Computational Chemistry Symposium (16) Biology II CHAIR: Emilia Sicilia, Hiroyuki Teramae (ROOM 2)		
15:20 – 15:45	<i>Yoong-Kee Choe</i>	Catalytic Conversion of Ethanol to Butadiene: A DFT Study of the Complex Reaction Mechanism
15:45 – 16:10	<i>Hiroyuki Teramae</i>	Ab Initio Electronic Structure Calculation of Polymononucleotide, a Model of B-type DNA
16:10 – 16:35	<i>Norifumi Yamamoto</i>	Theoretical Insights into the Aggregation-Induced Emission of a Cyanostilbene Derivative
16:35 – 16:55 (20 min)	<i>Toshio Asada</i>	COMPUTATIONAL APPROACH TO MOLECULAR DESIGN USING FREE ENERGY CONTRIBUTION ANALYSIS
16:55 – 17:05 (10 min)	<i>Takanori Matsumaru</i>	Chemical synthesis and signaling activity of conjugated lipids through C-type lectin receptor Mincle
Coffee Break (The coffee break will be available between 16:30 - 17:30)		



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16 March 2018		
SESSION: Modern Information Technology as an Instrument Used in Sport, Tourism and Recreation to Build a Healthy Society		
CHAIR: Mirosława Szark-Eckardt and Hanna Żukowska (ROOM 3)		
15:00 – 15:30	<i>Wiesława Pilewska</i>	<i>Sport and modern technologies</i>
15:30 – 16:00	Dominika Muszyńska-Jeleszyńska	The use of solar technology on vessels (boats) for development of water tourism and recreation - Bydgoszcz Water Tram case study
16:00 – 16:30	Żaneta Marciniak	The use of mobile application for development of water tourism and recreation – Żuławy Loop case study



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16 March 2018 SESSION 20: V International Symposium of Computational and Mathematical Modeling of Biology and Medicine Targets CHAIR: Dilson Silva (ROOM 4)		
15:00 – 15:30	<u><i>Francisco Albuquerque</i></u>	Modelling the Energy Balance and Turbulent Flows for Urban Surface Temperature Estimation Using the Improved Force Restore Technique
15:30 – 16:00	<u><i>Liliane Morais</i></u>	DNA Aptamer as Molecular Tool for ZIKV NS1 Protein Detection
16:00 – 16:30	<u><i>Lígia Tchaicka</i></u>	Molecular Differentiation of <i>Colletotrichum</i> spp. Associated with Tropical Fruit Anthracnose
16:30 – 17:00	<i>Audalio Torres</i>	The Eventual Presence of Freshwater of Amazonas River Over the Continental Shelf of the State of Maranhão – Brazil



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16 March 2018		
SESSION: Computational Chemistry Symposium (14)		
Light-Matter Interaction II		
CHAIR: Toshiyuki Takayanagi, Tomokazu Yasuike		
(ROOM 1)		
17:30 – 17:55	<i>Toshiyuki Takayanagi</i>	Quantum dynamics calculations of transition state spectra of gas-phase chemical reactions
17:55 – 18:20	<i>Heide Ibrahim</i>	Is there a difference when controlling the breakup channels in symmetric and asymmetric molecules?
18:20 – 18:45	<i>Himadri Pathak</i>	Time-dependent coupled-cluster method for laser-driven multielectron dynamics
18:45 – 19:10	<i>Tomokazu Yasuike</i>	Hot-carrier induced multidimensional nonequilibrium dynamics of adsorbate: CO desorption from Cu(100)
19:10 – 19:35	<i>Milan Milosevic</i>	Silicon Photonics at the University of Southampton



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16 March 2018 SESSION: Computational Chemistry Symposium (17) Materials III CHAIR: Koichi Yamashita (ROOM 2)		
17:30 – 17:55	<i>Alyona Starikova</i>	Computational insight into geometry, energetic and magnetic properties of the transition metal complexes with redox-active ligands: a DFT approach
17:55 – 18:20	<i>Fabio Denis Romero</i>	Sequential Charge Transitions in $\text{Ca}_{0.5}\text{Bi}_{0.5}\text{FeO}_3$ and the electronic consequences of B-site doping
18:20 – 18:45	<i>Satoru Iuchi</i>	Molecular dynamics simulations of light-induced spin crossover in an iron(II) complex: a model electronic Hamiltonian approach
18:45 – 19:10	<i>Eriko Sato</i>	Coumarin Derivative Polymers for Thermo- and Light-Responsive Monofunctional Polymers
19:10 – 19:35	<i>Eisuke Ohta</i>	Fluorescence Domain “Excited Multimer” Formed in Crystals of Diaroylmethanoboron Difluoride



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<p>16 March 2018</p> <p>SESSION: Challenges for computational methods in wellbeing and social science research.</p> <p>CHAIR: Prof. Anna Dluzewska, Prof. Rock Molz</p> <p>(ROOM 3)</p>		
<p>17:30 – 18:00</p>	<p><i>Dr Monika Kozłowska-Adamczak</i></p>	<p>The peripheral location of region of the versus processes of emerging the tourism space - selected methodological problems. Krajna (Poland) case studies.</p>
<p>18:00 – 18:30</p>	<p><i>Dr Alicja Gonja</i></p>	<p>The application of the modified multidimensional comparative method for assessing tourist potential as illustrated with the example of the Lower Vistula communes (Kuyavian-Pomeranian and Pomeranian voivodeships, Poland).</p>
<p>18:30 – 19:00</p>	<p><i>Prof. Anna Dluzewska</i></p>	<p>How can you know what's well for me? Gaps and challenges for wellbeing measuring and research.</p>



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16 March 2018 SESSION: Computational Chemistry Symposium (22) Oral Presentation CHAIR: Tokuei Sako (ROOM 1)		
21:00 – 21:10 (10 min)	<i>Shogo Kunieda</i>	Surface Structure Chemical Transfer (SSCT) Method for Fabrication of Low Reflectance and High Carrier Lifetime Textured Multi-Crystalline Silicon
21:10 – 21:20 (10 min)	<i>Hajime Suzuki</i>	Z-scheme water splitting using tungstic acids as oxygen-evolving photocatalysts under visible light
21:20 – 21:30 (10 min)	<i>Kohei Sasaki</i>	Influence of the point-charge modeling on the structure of mixtures of epoxy resin and amine-curing agent observed in molecular dynamics simulations
21:30 – 21:40 (10 min)	<i>Kento Suzuki</i>	Real-time nonadiabatic ionization dynamics of low-temperature helium clusters using ring-polymer MD method
21:40 – 21:50 (10 min)	<i>Eiki Ozama</i>	Path Integral Molecular Dynamics study on structures of Ac ³⁺ -doped helium clusters



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16 March 2018 Poster Session: The Information, Intelligent, Education and Engineering Application 15:00 - 17:00	
<u>Ying Liu and Cheng Lian</u>	Tentative Analysis of Tea Beverage Enterprise Patent Protection Strategy
<u>Yucheng Shen, Chialiang Lin and Yukuang Liu</u>	Comparison of Self-regulation between Students in Taiwan and Yunnan to Academic Performance
<u>Lungchiuan "Danny" Chiang</u>	Design and Testing of an Instrument to Measure Cultural Competence among College Seniors: A Preliminary Study
<u>Chialiang Lin and Jwujenq Chen</u>	The Operating Efficiency Evaluated System Development for Photovoltaic System Applying Multi-Axis Drone
<u>Xiaoyan Ye, Xiaoying Ye and Ruiran Wu</u>	Security Analysis of Yu-Cao Neural Networks Scheme
<u>Xiaoying Ye, Chenglian Liu and Donald Gardner</u>	Weakness of RSA Cryptosystem Characteristic

END OF THE 2ND DAY



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17 March 2018 SESSION: Computational Chemistry Symposium (19) Highlight V CHAIR: Cecilia Coletti (ROOM 1)		
9:35 – 10:00	<i>Roberto Cammi</i>	Quantum Chemistry at the high pressures: a new perspective based on the XP-PCM method.
Coffee Break		



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17 March 2018 SESSION: Plasmonics and Nanophotonics CHAIR: T. Gric (ROOM 1)		
08:00 – 08:15	<i>Ortwin Hess</i>	Active and chiral nanoplasmonic metamaterials
08:15 – 08:30	<i>Patrice Genevet</i>	Conformal optical metasurfaces and applications
08:30 – 08:45	<i>Wolfgang Fritzsche</i>	Single plasmonic nanoparticle for optical bioanalytics
08:45 – 09:00	<i>Jonas Fransson</i>	Voltage controlled magnetic interactions in coupled magnetic molecules
09:00 – 09:15	<i>Steve Smith</i>	Controlling Near-Infrared to Visible Upconversion with Plasmonic Surfaces
09:15 – 09:30	<i>Kofi Edee</i>	On some modal methods in photonics: from the Fourier modal method to the polynomial modal method
09:30 – 09:45	<i>Sergey Sekatskii</i>	Ultrasensitive optical bio- and gas sensors based on 1D Photonic Crystal – supported surface waves: experimental results and design principles
09:45 – 10:00	<i>Yaseen Naser Jurn</i>	Different Carbon Nanotubes Structures for Millimeter Wave Antenna Applications
10:00 – 10:15	<i>Aleksandr Cherniadev</i>	Investigation of terajets produced by dielectric parallelepiped structure
10:15 – 10:30	<i>Chan Jun</i>	High efficient photoluminescence by Surface plasmon enhancement in graphene quantum dot decorated metal-nanosphere



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17 March 2018 SESSION: Differential Equations CHAIR: Theodore Simos (ROOM 2)		
9:30 – 9:50	<i>Z. Kalogiratos, Th. Monovasilis, T.E.Simos</i>	Two Derivative Runge-Kutta method for the Schrodinger Equation
9:50 – 10:10	<i>Th. Monovasilis, Z. Kalogiratos, T.E.Simos</i>	Comparison of Two-Derivative Runge-Kutta methods



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17 March 2018

11:00 – 18:00

CENTRAL EXCURSION

17 March 2018

20:30 – 24:00

CENTEAL DINNER

END OF THE 3RD DAY



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18 March 2018 SESSION: Computational Chemistry Symposium (20) Highlight VI, Light-Matter Interaction III CHAIR: Nils Schopohl (ROOM 1)		
9:15 – 9:40	<i>Tomoya Okino</i>	Observation of ultrafast molecular dynamics with a-few-pulse attosecond pulse train
9:40 – 10:05	<i>Constantin Meis</i>	The single photon state, the quantum vacuum and the elementary electron/positron charges.
10:05 – 10:30	<i>Yasushi Kino</i>	Bound and Resonance States of Positronic Alkali Atoms
Coffee Break (The coffee break will be available between 10:30 - 11:30)		



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18 March 2018 SESSION: Modelling, estimation and control for distributed finance systems CHAIR: G. Rigatos, P. Siano and T. Ghosh (ROOM 2)		
09:00 – 09:30	<i>G. Rigatos, P. Siano, T. Ghosh and N. Zervos</i>	Nonlinear optimal control for the IS-LM business cycles model under time-delays
09:30 – 10:00	<i>G. Rigatos, P. Siano, V. Loia and T. Ghosh</i>	Statistical validation of multi-agent financial models using the H-infinity Kalman Filter
10:00 – 10:30	<i>G. Rigatos, P. Siano, T. Ghosh and V. Ding</i>	Forecasting of commodities prices using a multi-factor PDE model and Kalman Filtering
10:30 – 11:00	<i>G. Rigatos, P. Siano and T. Ghosh and A. Krawiec</i>	Nonlinear optimal control for a business cycles macroeconomic model of linked economies
11:00 – 11:30	Coffee Break (The coffee breaks will be available between 16:30 - 17:30)	



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18 March 2018 MS15: Existing and New Structures in Seismic Prone Areas: Advanced Numerical Modelling and Experimentation CHAIR: F. Clementi, G. Milani, A. Formisano (ROOM 3)		
09:00 – 09:25	<u><i>Tiberti S.,</i></u> <u><i>Macorini L.,</i></u> <u><i>Milani G.</i></u>	Homogenized ultimate behavior of rubble masonry
09:25 – 09:50	<u><i>Bertolesi E.,</i></u> <u><i>Milani G., Grande E.,</i></u> <u><i>Fagone M., Rotunno T.</i></u>	Delamination of FRP reinforced curved masonry pillars: experimentation and advanced numerical analyses
09:50 – 10:15	<u><i>Olivito R.S.,</i></u> <u><i>Porzio S., Scuro C.,</i></u> <u><i>Codispoti R.</i></u>	Evaluations on the Seismic Vulnerability of Masonry Churches: a case study in Amantea (Cosenza – Italy)
10:15 – 10:40	<u><i>Stockdale G.,</i></u> <u><i>Milani G.</i></u>	AutoLisp Interactive Upper-Bound limit analysis of masonry arches



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18 March 2018 SESSION: General Session CHAIR: Zsolt Horváth (ROOM 4)		
09:30 – 10:00	<u>G. D’Alessio, G. Aversano, Z. Li and A. Parente</u>	Feature Extraction by means of Unsupervised Learning Techniques on LES Combustion Data
10:00 – 10:30	<u>Zsolt Horváth, Petra Csomós</u>	A Switched Linear System Approach to the Modeling of the Air Path of Diesel Engines
10:30 – 11:00	<u>Yipeng Ge, Maximilian Hansinger, Christoph Traxinger and Michael Pfitzner</u>	Deep Residual Learning applied to real-gas thermodynamics



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18 March 2018 SESSION: Computational Chemistry Symposium (21) Highlight VII CHAIR: Roberto Cammi (ROOM 1)		
11:00 – 11:25	<i>Ken Onda</i>	Structural Dynamics in Photofunctional Materials Studied by Time-resolved Infrared Vibrational Spectroscopy
11:25 – 11:50	<i>Nathalie Guihéry</i>	Study of the Electronic Structure of NiGa₂S₄ and Extraction of the Spin Hamiltonian Parameters from <i>Ab Initio</i> Calculations
11:50 – 12:15	<i>Noam Agmon</i>	A theoretical estimate for the radii of cations with spherically symmetric charge distribution
12:15 – 12:40	<i>Gabriel Hanna</i>	Modeling heat transfer at the nanoscale: A mixed quantum-classical approach
Lunch Break		
14:00-18:00	Free Discussion	



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18 March 2018 SESSION: Modelling, estimation and control for distributed finance systems CHAIR: G. Rigatos, P. Siano and T. Ghosh (ROOM 2)		
11:30 – 12:00	<i>G. Rigatos, P. Siano and T. Ghosh and B. Xin</i>	Nonlinear optimal control of industrial production under an oligopolies model
12:00 – 12:30	<i>G. Rigatos, P. Siano and T. Ghosh</i>	Stabilization of a stock-loan valuation PDE process using differential flatness theory



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18 March 2018 SESSION: General Session CHAIR: Miguel Hermanns (ROOM 3)		
11:30 – 12:00	<u><i>Ernestos Sarris,</i></u> <i>Abdullahi Aladeyelu</i> <i>and Elias Gravanis</i>	The Influence of Diffusion in the Fracture Resistance Method for Wellbore Strengthening: A Rock Mechanics Approach
12:00 – 12:30	<i>Miguel Hermanns</i>	An Order 10² Speedup in the Computation of the Steady-State Thermal Response of Geothermal Heat Exchangers
12:30 – 13:00	<u><i>Ilka Márcia Ribeiro de Souza Serra,</i></u> <i>Karina Cristina Silva Braga,</i> <i>Lígia Tchaickaand</i> <i>Thiago Anchieta de Melo</i>	Molecular Differentiation of Colletotrichum spp. Associated with Tropical FruitAnthracnose
13:00 – 13:30	<u><i>G. Aversano,</i></u> <i>Z. Li, O. Gicquel</i> <i>and A. Parente</i>	Model Reduction by PCA and Kriging



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18 March 2018 SESSION: General Session CHAIR: Vladislav N. Kovalnogov (ROOM 4)		
11:30 – 12:00	<i><u>Yury E. Chamchiyan,</u> <u>Vladislav N.</u> <u>Kovalnogov,</u> and <u>Dmitry V. Suranov</u> </i>	Modeling, Research and Development of Technical Properties of Exterior Walls and PVC Windows to Influence Building Microclimate
12:00 – 12:30	<i><u>Ruslan V. Fedorov,</u> <u>Vladislav N.</u> <u>Kovalnogov,</u> <u>Igor A. Maleshin,</u> <u>Andrey V. Tamyarov,</u> <u>Maya V. Tamyarova,</u> <u>and</u> <u>Andrey I. Tikhonov</u> </i>	Technology of Designing Energy Efficient Power Converters on the Basis of Programmable Field Models
12:30 – 13:00	<i><u>Vladislav N.</u> <u>Kovalnogov,</u> <u>Mikhail S. Boyarkin,</u> <u>Tamara V. Karpukhina,</u> <u>Maxim G. Korniliev,</u> <u>and</u> <u>Ruslan V. Fedorov</u> </i>	Modeling and Investigation of the Intensification of Fluid Diffusion in the Capillary-Porous Space by Applying Periodic Pressure Pulsations



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18 March 2018 Poster Session of the Second Symposium on Computational Methods in Economics and Nature Use CHAIR: Alexander Medvedev, Marina Medvedeva 11:30 – 12:30	
<u><i>Ershov A.A.,</i></u> <u><i>Tsoi V.K.,</i></u> <u><i>Ushakov A.V.</i></u>	Sufficient Conditions for Effective Application of the Runge-Kutta Method for Construction of Reachability Sets of Control Systems
<u><i>Ushakov V.N.,</i></u> <u><i>Matviychuk A.R., Ushakov</i></u> <u><i>A.V.</i></u>	Problems of Game Control on Finite Time Interval
<u><i>Alexandr A. Tarasyev,</i></u> <u><i>Gavriil A. Agarkov,</i></u> <u><i>Seyed Iman Hosseini</i></u>	Application of Machine Learning Methods to Migrant Behaviour Modeling
<u><i>Gavriil A. Agarkov, Viktor</i></u> <u><i>A. Koksharov</i></u>	Data Mining Algorithms for Modeling International Scientific Migration
<u><i>Alexandr A. Tarasyev,</i></u> <u><i>Gavriil A. Agarkov</i></u>	Dynamic Modeling of Scientific Migration in Terms of Proportional Economic Growth
<u><i>Shichkin A.V., Buevich</i></u> <u><i>A.G., Sergeev A.P.,</i></u> <u><i>Baglaeva E. M.,</i></u> <u><i>Subbotina I.E.</i></u>	Forecasting of Spatial Variable by the Models Based on Artificial Neural Networks on an Example of Heavy Metal Content in Topsoil
<u><i>Baglaeva E.M., Buevich</i></u> <u><i>A.G., Sergeev A.P.,</i></u> <u><i>Shichkin A.V., Subbotina</i></u> <u><i>I.E.</i></u>	Recognition of Chromium Distribution Features in Different Urban Soils by Multilayer Perceptron
<u><i>Buevich A.G., Shichkin</i></u> <u><i>A.V., Sergeev A.P.,</i></u> <u><i>Antonov K.L.,</i></u> <u><i>Sergeeva M.V.</i></u>	Analysis of time series of greenhouse gas concentrations in the Russian Arctic using the artificial neural networks



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<u><i>Varaksin A.N., Rylova A.P., Detkov .A., Ilysheva M.A.</i></u>	Regression models of macroeconomic paradoxes: the case of Inflation and the Interest Rate in Russia
<u><i>Alexander M. Tarasyev, Julian Vasilev, Victoria F. Turygina</i></u>	Statistical Analysis and Forecasting of Extraction and Use of Natural Resources
<u><i>Nikolay A. Krasovskii, Alexander M. Tarasyev</i></u>	Models of Energy Infrastructure and Dynamical Coordination Games
<u><i>Anton Panachev, Evgeny Komotskiy, Dmitry Berg</i></u>	Prediction of Ferrous Scrap Price: Neural Network Model Application
<u><i>Dmitry Berg, Mariya Demina, Ksenia Isaychik, Anton Panachev, Valerian Popkov</i></u>	Competition of Payment Systems in Russia: Numerical Analysis
<u><i>Valery Kalinin, Dmitry Berg, Valerian Popkov, Julia Nazarova</i></u>	R/S-analysis of cash-flow: cases of business eco community and separate enterprise
<u><i>Bozhko Yu.O., Lavrinenko T.V., Medvedev M.A., Gizatulin A.M.</i></u>	Imitation Model for Assessing the Resource-Technological Potential of an Industrial Enterprise
<u><i>Igor N. Sachkov, Viktoria F. Turygina, Maxim A. Medvedev, Aleksey N. Dolganov</i></u>	Development of new FEM programs for synergistic evaporation processes from porous systems



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18 March 2018 Poster Session of the Second Symposium on Computational Methods in Economics and Nature Use CHAIR: Alexander Medvedev, Marina Medvedeva 15:00 – 16:00	
<u>Anna Kolomytseva,</u> <u>Marina Medvedeva,</u> <u>Malika Lutfullaeva, Vitaly</u> <u>Kolomiets</u>	Application of Information Systems Aimed at Big Data Use in the Sphere of State Finance Management: a Concept Scheme
<u>Iskra E.A., Medvedeva</u> <u>M.A., Apanasenko A.V.</u>	An integrated model of efficiency analysis of companies network interaction
<u>V.A. Poddubny,</u> <u>E.S. Dubinkina,</u> <u>J.I. Markelov,</u> <u>A.G. Buevich,</u> <u>K.L. Antonov,</u> <u>E.V. Omelkova,</u> <u>I.L. Manzhurov,</u> <u>A.N. Medvedev</u>	Recovery of the Average Effective Methane Concentration Field in the Region of the Kara and Barents Seas Using a Passive Location of the Atmosphere by the Wind
<u>Ayshan Gasanova,</u> <u>Alexander N. Medvedev,</u> <u>Evgeny I. Komotskiy</u>	On the Use of Data Mining Methods for the Money Laundering Detection Based on Financial Transactions Information

END OF THE 4TH DAY
END OF THE CONFERENCE