



PLEASE ATTENTION

The Desk of the Conference will be open for Registration, Requests etc the following days and hours:

Sunday 02/10/2010 14:00 – 17:00

Monday 03/10/2010 10:00 – 13:00 and 17:30 – 19:30

Tuesday 04/10/2010 10:00 – 13:00 and 17:30 – 19:30

Wednesday 05/10/2010 10:00 – 12:30

Thursday 06/10/2010 10:30 – 12:30

Friday 07/10/2010 10:30 – 12:30



<p align="center">02 October 2011 SESSION 5: 8th Symposium on Industrial and Environmental Case Studies CHAIR: Christina G. Siontorou (ROOM 1)</p>		
14:30 – 14:45	<i>GIS based simulation of the photovoltaic systems diffusion: the case of Greece</i>	M. Roditi
14:45 – 15:00	<i>Applying a modified contingent valuation method (CVM) for the preservation/ restoration of the lake Kastoria in northern Greece</i>	E. Zoupanidou
15:00 – 15:15	<i>Contribution to individualized environmental education</i>	A. Karagiannopoulou
15:15 – 15:30	<i>On the design of biosensor arrays with techno-economic criteria</i>	C. Siontorou
15:30 – 15:45	<i>Optimal design of a biomass-packed-bed column for toxic metals removal / recovery from aquatic solutions</i>	D. Politi
15:45 – 16:00	<i>Development of a knowledge base for optimizing ballast seawater processing</i>	M. Psoma
16:00 – 16:15	<i>Knowledge acquisition for reconstruction and identification of</i>	O. Kopsidas



	<i>dimensionless groups by means of case based reasoning</i>	
16:15 – 16:30	<i>An algorithmic procedure for the design of severity factor in biomass pretreatment for adsorption</i>	A. Mathioudaki

Poster Session:

- *Interconnecting GIS layers as a means for pollution propagation/
differentiation mapping in water bodies.*
S. Giakoumatos & C. Siontorou
- *A polynomial model for estimating scale economies in biogas
production units*
D. Batzias
- *Study on the effect of an oil dispersant on a simulated seawater
column sedimentation*
D. Sidiras, V. Giannopoulos & I. Konstantinou
- *Incorporating logistics in an industrial ecology framework for
minimizing environmental impact under economic constraints*
A. Bountri, A. Mathioudaki
- *Using raw chickpeas straw as a low-cost adsorbent of methylene blue*
M. Margoni, A. Geronti & D. Sidiras
- *On the relation between externalities and industrial ecology in the
case of pollution abatement*
F. Batzias & K. Kondyla
- *Investigating the problem of parameter identification when
combining thermodynamic and kinetic parameters within the same
model*
A. Bountri & K. Bardi
- *A knowledge based multidisciplinary taxonomy of industrial dyes for
solving the problem of wastewater decolorization*
C. Siontorou & A. Bountri



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G-Hotels, Halkidiki, Greece, 02-07 October 2011

02 October 2011		
SESSION: MATHEMATICAL METHODS		
CHAIRS:		
(ROOM 1)		
17:00 – 17:30	<i>Metin Demiralp and Emre Demiralp</i>	Probabilistic Evolutions: The Ultimate, Natural and Exact Linearisation of ODEs
17:30 – 18:00	<i>Metin Demiralp and Emre Demiralp</i>	Increasing the Qualities of the Truncated Probabilistic Evolutions by Controlling Fluctuations
18:00 – 18:30	<i>Ercan Gürvit, N. A. Baykara and M. Demiralp</i>	Employing the Probabilistic Evolutions of ODEs in Function Inversion under Fluctuation Control
18:30 – 19:00	<i>N. Abdölbaki Baykara, Ercan Gürvit and M. Demiralp</i>	Axial and Planar Probabilistic Evolutions in Explicit Ordinary Differential Equations
19:00 – 19:30	<i>Emre Demiralp and Metin Demiralp</i>	Constrained Parameter Estimation in Dynamical Systems



03 October 2011 SESSION: COMPUTATIONAL QUANTUM CHEMISTRY CHAIR: George Maroulis (ROOM 1)		
09:00 – 09:50	<i>Yuriko Aoki</i>	Highly accurate functional design of DNA/Nanotubes/Nanowires by efficient quantum chemical approach
09:50 – 10:35	<i>Gilberte Chambaud</i>	From atoms to nanowires: a model for the surface effects
Coffee Break		
03 October 2011 SESSION: COMPUTATIONAL QUANTUM CHEMISTRY CHAIR: Yuriko Aoki (ROOM 1)		
14:30 – 15:15	<i>Masayoshi Nakano</i>	Open-Shell Supermolecular Systems Composed of Phenalenyl Radical Units: Open-Shell Characters and Third-Order Nonlinear Optical Properties
15:15 – 15:50	<i>David Cappelletti</i>	Hydrogen and Halogen Bonding in Gas Phase Complexes of Water
15:50 – 16:25	<i>Philippe Carbonière</i>	Methodological development and algorithms for the computation of structural and vibrational properties: molecules and clusters
16:25 – 17:00	<i>Feng-Long Gu</i>	Nonlinear Optical Properties for Large Systems: Elongation Method towards Linear Scaling



03 October 2011 SESSION: CHEMICAL MODELLING CHAIRS: George Maroulis/Mihai V. Putz (ROOM 2)		
09:00 – 09:15	MIHAI V. PUTZ	<i>On The Orthogonal Space of Chemical Reactivity</i>
09:15 – 10:00	JAN C.A. BOEYENS	<i>Chemical Modeling by Number Theory</i>
10:20 – 10:50	PAUL MEZEY	<i>Modeling Molecular Property Variations in Conformational Ranges</i>
Coffee Break		
10:50 – 11:20	MARIA BELEN RUIZ	<i>Atomic Excitations During Nuclear B-Decay Processes In Light Atoms</i>

Poster Session 09:00 – 12:00	
<i>Ana Maria PUTZ,</i> <i>Cecilia SAVII</i>	Modelling mesoporous silica materials properties applied as drug carriers
<i>Hanmei E</i>	Study on Educational Management Information Systems Based On Data Mining



04 October 2011 SESSION 1: Optics and magneto-optics CHAIR: S. A. Mikhailov (ROOM 1)		
09:00 – 09:40	S. D. Ganichev, <i>University of Regensburg, Germany</i>	Photon helicity dependent electric currents in graphene
09:40 – 10:10	L.A. Falkovsky, <i>Landau Institute for Theoretical Physics, Russia</i>	Quantum magneto-optics of graphite with trigonal warping
10:10 – 10:40	I. Crassee, <i>Université de Genève, Switzerland</i>	Anomalies in the magneto-optical conductivities of multilayer epitaxial graphene
10:40 – 11:10	M. Orlita, <i>High Magnetic Field Lab. Grenoble, France</i>	Cyclotron motion in the vicinity of Lifshitz transition in graphite
Coffee Break		
SESSION 2: Nonlinear phenomena CHAIR: L. A. Falkovsky (ROOM 1)		
11:30 – 12:10	S. A. Mikhailov, <i>University of Augsburg, Germany</i>	Plasma effects in the higher harmonics generation in graphene
12:10 – 12:40	R. J. Stöhr, <i>University of Stuttgart, Germany</i>	Non-linear optical response from graphene under pulsed laser excitation
12:40 – 13:10	K. Yoneda, <i>Osaka University, Japan</i>	Open-shell characters, aromaticities and second hyperpolarizabilities for hexagonal graphene nanoflakes with antidot structures
Lunch		
SESSION 3: Plasmons and solitons CHAIR: S. D. Ganichev (ROOM 1)		
15:30 – 16:00	Shengjun Yuan, <i>Radboud University of Nijmegen, The Netherlands</i>	Excitation spectrum and high energy plasmons in single- and multi-layer graphene
16:00 – 16:30	F. Biancalana, <i>Max Planck Institute for the Science of Light, Erlangen, Germany</i>	Terahertz relativistic spatial solitons in doped graphene metamaterials



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16:30 – 17:00	T. Tudorovskiy, <i>Radboud University of Nijmegen, The Netherlands</i>	Inter-valley plasmons in graphene
17:00 – 17:30	F. Koppens, <i>Institute of photonic sciences, Barselona, Spain</i>	Graphene nano-optoelectronics and plasmonics
Coffee Break		
SESSION 4: Raman scattering CHAIR: S. A. Mikhailov (ROOM 1)		
18:00 – 18:40	M. Potemski, <i>High Magnetic Field Lab. Grenoble, France</i>	Magneto-Raman scattering of graphene and graphite: Electronic and E_{2g}-phonon excitations
18:40 – 18:50	Closing	of Symposium



04 October 2011 SESSION: COMPUTATIONAL QUANTUM CHEMISTRY CHAIR: Masayoshi Nakano (ROOM 2)		
09:00 – 09:45	<i>Mitsutaka Okumura</i>	Theoretical investigation of the hetero-junction effect in Precious metal cluster systems
09:45 – 10:25	<i>Hirofumi Sakai</i>	All-optical molecular orientation and future challenges
10:25 – 11:00	<i>Magnus Gustaffson</i>	Radiative broadening of long-lived quasibound states
Coffee Break		
11:35 – 12:10	<i>Panagiotis Karamanis</i>	(Hyper)polarizabilities of alkali-metal-functionalized clusters
Lunch Break		
04 October 2011 SESSION: COMPUTATIONAL QUANTUM CHEMISTRY CHAIR: Xavier Assfeld (ROOM 2)		
14:30 – 15:15	<i>Shigeyoshi Sakaki</i>	C-H sigma-Bond Activation and Catalytic Reaction by Transition Metal Complexes. A Theoretical Study
15:15 – 15:50	<i>Takashi Kubo</i>	Singlet Open-Shell Character of Conjugated Kekulé Molecules
15:50 – 16:25	<i>Marianna Safronova</i>	Coupled-cluster method for atomic clock research
16:25 – 17:00	<i>Yasuteru Shigeta</i>	First-principles analyses on reaction mechanisms of enzymes and related topics



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17:00 – 17:25	<i>Takuya Minami</i>	Tuned Long Range Corrected Density Functional Theory Study of the Excited States on Pentacene/C ₆₀
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05 October 2011 SESSION: INVITED SPEAKER CHAIR: Marianna Safronova (ROOM 1)		
10:00 – 11:00	David Logan	Correlated electrons on the nanoscale

05 October 2011
11:30 Excursion

05 October 2011
<u>19:30</u> Dinner



06 October 2011		
SESSION: COMPUTATIONAL METHODS I		
CHAIRS: Ken-ichi Sugiura		
(ROOM 1)		
10:00 – 10:30	<i>Martin Kabeláč and Adam Pecina</i>	Ability Of Semiempirical Methods To Describe Interactions Of Biomolecules With Ions
10:30 – 11:00	<i>H. Tanimura, Y. Honda, K. Sugiura, and <u>M. Hada</u></i>	NMR chemical shifts and Aromaticity of Cyclic π-electron Systems
11:00 – 11:30	<i><u>Ken-ichi Sugiura</u>, Ken-ichi Yamashita, Motoko S. Asano, and Masahiko Hada</i>	Syntheses and Photochemistries of Shape Persistent Macrocycles Based on Porphyrin and Pyrene
11:30 – 12:00	<i>B. Soltanalizadeh and Ahmet Yildirim</i>	An efficient technique for Sobolev-type differential equation with nonlocal boundary conditions
12:00 – 12:30	<i>Guido Ala, Gianpiero Di Blasi and Elisa Francomano</i>	An advanced numerical method to simulate human brain activity
12:30 – 13:00	<i>Bogdan Lipuš and Borut Žalik</i>	The effects of points modification on lossy LAS file compression



07 October 2011 SESSION: COMPUTATIONAL METHODS II CHAIRS: V. Loukopoulos (ROOM 1)		
10:00 – 10:30	<i>G. Papakaliatakis and D. Mentou</i>	The influence of the adjacent fibres on debonding arrest of a broken fibre in SiC/Al composites with a 3D model
10:30 – 11:00	<i>G.A.T. Messaris, C.A. Papastavrou, V.C. Loukopoulos and G.T. Karahalios</i>	An approximate numerical solution giving the wall shear stress for pulsatile flow in a curved pipe
11:00 – 11:30	<i>Deepinderdeep Kaur and Sukesha</i>	Wireless Sensor Networks: Reduced Delay And Energy Efficient MAC Protocols And Their Comparison
11:30 – 12:00	<i>Lakshmi Deepika C., Kandaswamy A., Vimal C., Arun R.</i>	Probabilistic Classifier for Palmprint Recognition using Bayesian Belief Networks