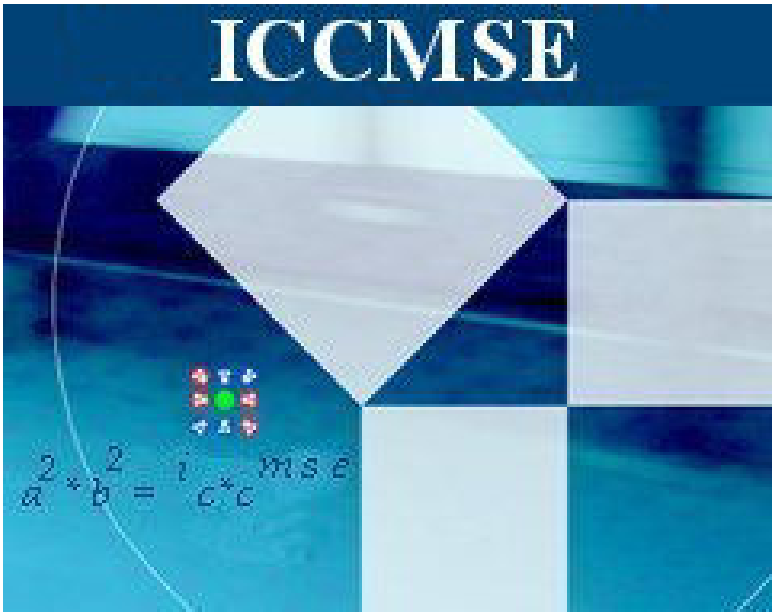
ICCMSE 2006



PROGRAM

27 October – 1 November 2006

CONFERENCE CENTER:

HOTEL PANORAMA, CHANIA, CRETE, GREECE

Under the Auspices of

- European Society of Computational Methods in Sciences and Engineering (ESCMCE)

Chairmen and Organizers

Prof. T.E. Simos, President of ESCMSE, Member of the Presidium of the European Academy of Sciences, Active Member of the European Academy of Sciences and Arts and Corresponding Member of the European Academy of Sciences, Corresponding Member of the European Academy of Arts, Sciences and Humanities, Department of Computer Science and Technology, Faculty of Sciences and Technology, University of Peloponnese, GR-221 00 Tripolis, Greece.

Prof. George Maroulis, Co-Chairman, Computational Quantum Chemistry Research Group, Department of Chemistry, Department of Chemistry, University of Patras, GR-26500 Patras, Greece

Scientific Committee:

Dr. B. Champagne, Université de Namur, Belgique

Prof. S. Farantos, University of Crete, Greece

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Dr. G. Psihoyios, Vice-President ESCMSE

Prof. B. M. Rode, University of Innsbruck, Austria.

Prof. A. J. Thakkar, University of New Brunswick, Canada

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Mr. G. Vourganas
Mr. Th. Monovasilis
Mr. Constantinos Makris

THURSDAY 26 OCTOBER 2006

21:30 – 23:00

INFORMAL WELCOME DRINK

FRIDAY 27 OCTOBER 2006

09:50 – 10:00 (ROOM 1)

OPENING CEREMONY

PLEASE ATTENTION

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

Thursday 26/10/06: 18.00 – 21.00
Friday 27/10/06: 09:00 – 13:00, 15:00 – 20:00
Saturday 28/10/06: 09:00–13:00, 15:00-20:00
Sunday 29/10/06: 10:00 – 13:00
Monday 30/10/06: 09:00–13:00, 16:30 – 20:00
Tuesday 31/10/06: 09:00–13:00, 16:30 –20:00
Wednesday 1/11/06:09:00–13:00, 16:30-20:00

ELECTRON CORRELATION FOR THE WHOLE PERIODIC TABLE

A theoretical chemistry Symposium in honour of Björn O. Roos
Crete, October 27-29 2006
Friday October 27, 2006 (Room 1)

Schedule	Speaker	Title of the contribution
10.15 - 10.30	Laura Gagliardi, Geneva, Switzerland	*OPENING*
	Chair	*Aristides D. Zdetsis*
10.30 - 11.00	Peter R. Taylor, Warwick, Coventry, UK	*How do we treat electron correlation in small carbon rings?*
11.00 - 11.30	Kristine Pierloot, Leuven, Belgium	*Theoretical modeling of the relative spin-state energetics in transition-metal compounds : how accurate is CASPT2?*
11.30 - 12.00	**COFFEE BREAK**	
12.00 - 12.30	Kimihiko Hirao, Tokyo, Japan	*Photoelectron spectra of $Re(CO)_5X$ (X=Cl, Br, and I): CASPT2, SAC-CI, and DFT study*
12.30 - 13.00	Trygve Helgaker, Oslo, Norway	*Self-consistent field methods applied to large molecular systems*
LUNCH		
	Chair	*Stavros Farantos*
16.00 - 16.30	Ursula Roethlisberger, Lausanne, Switzerland	*Dispersion-Corrected Density Functional*
16.30 - 17.00	Margareta Blomberg, Stockholm, Sweden	*Modeling reactions of cytochrome c oxidase : Proton pumping and reduction of molecular oxygen and nitric oxide*
17.00 - 17.30	Marco Garavelli, Bologna, Italy	*Spectral tuning and photochemical reactivity control in biological chromophores : towards an accurate computational photobiology*
17.30 - 18.00	**COFFEE BREAK**	
18.00 - 18.30	Spiridoula Matsika, Temple, Philadelphia, USA	*Electronically excited states and conical intersections of complex systems using high level ab initio methods*
18.30 - 19.00	Roland Lindh, Lund, Sweden	*Cholesky decomposition of the two-electron integrals : A reliable tool for linear scaling methods?*

Friday 27 October 2006 SESSION: MATHEMATICAL AND COMPUTATIONAL METHODS CHAIR: METIN DEMIRALP (ROOM 2)		
10:15 – 10:45	*V. Artamonov, S. Sànchez*	**A mathematical classification for symmetries in 2-dimensional quasicrystals**
10:45 – 11:15	*A. Kalauzi, M. Cukic, H. M. Vega, S. Bonafoni, R. Biondi*	**Fractal Rhythms and Trends of Rainfall Data from Pastaza Province, Ecuador and Veneto, Italy**
11:15 – 11:45	*S. V. Kolomeiko, D. V. Mogilenskikh*	**One Algorithm of Approximation and 3D visualization of Objects Specified Combinatorially**
Coffee Break		
12.15 – 12:45	*M. Demiralp*	**Transformational High Dimensional Model Representation**
12:45 – 13:15	*Ana Mafalda Martins and António Leslie Bajuelos*	**Guarding two Subclasses of Orthogonal Polygons**
13:15 – 13:45	*D. Güvenç and M. Demiralp*	**High Dimensional Model Representation Based Partitioning of a Function's Data Set With Uncertainty in Data Given Points**

COMPUTATIONAL BIOLOGY: NETWORKS – THE LANGUAGE OF LIFE

Friday October 27 2006 (Room 2)

Schedule	**Speaker**	**Title of Contribution**
	Chair	*Danail G. Bonchev*
15:30 – 16:00	Gregory A. Buck, Richmond, USA.	Genomes to Networks, Pathways and Function
16:00 – 16:30	Jason Papin, Charlottesville, USA	Integrating Transcriptional Regulatory Reconstructions with Metabolic and Signaling Processes
16:30 – 17:00	Michael P. H. Stumpf, London, UK	Inferences form Noisy and Incomplete Biological Network Data
17:00 – 17:30		**Coffee Break**
	Chair	*Gregory A. Buck*
17:30 – 18:00	Vladimir A. Kuznetsov, Singapore	Emergence of Size-Dependent Networks on Genome Scale
18:00 – 18-30	Danail Bonchev, Richmond, USA	Cellular Automata (CA) As a Basic Method for Studying Network Dynamics

Friday 27 October 2006 SESSION: COMPUTATIONAL, NUMERICAL METHODS AND MODELLING CHAIR: J. M-S. LUBUMA (ROOM 3)		
10:15 – 10:45	*R. Anguelov, J. K. Djoko, P. Kama and J. M-S. Lubuma*	**On Elementary Stable and Dissipative Non-standard Finite Difference Schemes for Dynamical Systems**
10:45 – 11:15	*Khalid Alhumaizi & Mousatfa A. Soliman*	**An efficient collocation Method for Diffusion-Convection Problem with Chemical reaction**
11:15 – 11:45	*J. Biazar*	**Adomian Decomposition for concrete Examples**
Coffee Break		
12.15 – 12:45	*Guang-Hui Cheng, Ting-Zhu Huang*	**Relaxed alternating methods for Hermitian positive definite matrices**
12:45 – 13:15	*V. Dolejší*	**Numerical simulation of compressible flows with the aid of the BDF - DGFE scheme**

Friday 27 October 2006

SESSION: COMPUTATIONAL, NUMERICAL METHODS AND MODELLING
CHAIR:
C. KOUTITAS (ROOM 3)

15:30 – 16:00	*E. M. Fedriani and A. F. Tenorio*	**Algorithms to compute autonomous sets and fundamental products in Input-Output matrices**
16:00 – 16:30	*C. Koutitas and M. Gousidou-Koutita*	**A Numerical Model of Wave Energy Harnessing by Floating Breakwaters**
16:30 – 17:00	*Jonathan I. Matondo*	**Computational Methods Used to Generate Information Required in Climate Change Studies in Swaziland**
Coffee Break		
17.30 – 18:00	*M. Rizea*	**Improved Crank-Nicolson method applied to quantum tunnelling**
18:00 – 18:30	*Yunqing Yu, Kensuke Baba, Hanmei E, and Kazuaki Murakami*	**Bit-parallel Computation for String Alignment**
18:30 – 19:00	*Seongjai Kim*	**An Essentially Non-Oscillatory Crank-Nicolson Procedure for Incompressible Navier-Stokes Equations**
19:00 – 19:30	*Chaofeng Shi*	**A new self-adaptive algorithm for solving general mixed variational inequalities**
19:30 – 20:00	*Ahmad T. Jameel and Ashutosh Sharma*	**An Efficient Numerical Algorithm for the Solution of Nonlinear Problems with Periodic Boundary Conditions**

Friday 27 October 2006 SESSION: COMPUTATIONAL METHODS CHAIR: M. E. GRUNER (ROOM 4)		
10:15 – 10:45	*Ana M. Amado, S. M. Fiuza, L .A .E. Batista de Carvalho and M. P. M. Marques*	**Ab initio Conformational Study of Platinum and Palladium Complexes Towards the Understanding of the Potential Anticancer Activities**
10:45 – 11:15	*M. C. Gómez, V. Tchijov, F. León and A. Aguilar*	**Application of FEOM to chemical reaction mechanisms used in the 3D model of diffusion/advection of pollutants**
11:15 – 11:45	*M. E. Gruner, G. Rollmann, A. Hucht and P. Entel*	**Massively Parallel Density Functional Theory Calculations of Large Transition Metal Clusters**
Coffee Break		
12.15 – 12:45	*J. Czernek*	**Base Pairing Motifs Involving 1,8-Naphthyridine: an *ab Initio* Study**
12:45 – 13:15	*W. Győrffy, T. M. Henderson, and J. C. Greer*	**Statistical Estimates of Electron Correlations**
13:15 – 13:45	*Ji Eun Cho, Cheol Ho Choi*	**Theoretical Study of the thermal decomposition of primary thiols on the Si(100)-2X1 surface**

Friday 27 October 2006 SESSION: COMPUTATIONAL METHODS CHAIR: K. YAMAGUCHI (ROOM 4)		
15:30 – 16:00	*Thomas M. Henderson, Giorgos Fagas, Eoin Hyde, James C. Greer*	***Ab Initio* Complex Absorbing Potentials**
16:00 – 16:30	*Petra Ruth Kápralová-Ždánská and Jan Lazebníček*	**Potential scattering with varying projectile flux near metastable levels**
16:30 – 17:00	*K. Koizumi, M. Shoji, Y. Kitagawa, H. Isobe, R. Takeda, S. Yamanaka and K. Yamaguchi*	**Hybrid-DFT study on the high-valent metal-oxo bonds in manganese porphyrins and related species**
Coffee Break		
17.30 – 18:00	*N. Faginas Lago and A. Laganà*	**A Semiclassical Initial Value Representation Approach to $N + N_2$ Rate Coefficient**
18:00 – 18:30	*Joanna Makowska, Mariusz Makowski, Lech Chmurzyński*	**Theoretical Studies on the Alanine-rich Peptide**
18:30 – 19:00	*Davood Nori-Shargh, Fatemeh-Rozita Ghizadeh, Maryam Malekhosseini and Farzad Deyhimi*	**Configurational and Conformational Properties of Cyclododeca-1,2,7,8-tetraene: An Ab Inito Study and NBO Analysis**
19:00 – 19:30	*M. Shoji, K. Koizumi, Y. Kitagawa, T. Kawakami, S. Yamanaka, M. Okumura, K. Yamaguchi*	**Theoretical study on the electronic structure of [4Fe-4S] cluster**

Friday 27 October 2006 SESSION: COMPUTATIONAL METHODS CHAIR: T. TSUNEDA (ROOM 5)		
10:15 – 10:45	*T. Toraishi, T. Tsuneda, S. Tanaka*	**Mechanisms of Energy Transfer Luminescence of Lanthanide Complexes: A Time-Dependent Density Functional Theory Study**
10:45 – 11:15	*Carolina Tabares-Mendoza, Patricia Guadarrama*	**Predicting the catalytic efficiency by quantum-chemical descriptors. Theoretical study of pincer metallic complexes involved in the catalytic Heck reaction**
11:15 – 11:45	*X. Tan, G. Ouyang, G. W. Yang*	**Catalytic self-poisoning and bond-breaking selectivity at Ni step**
Coffee Break		
12.15 – 12:45	*DeCarlos E. Taylor, V. V. Karasiev, Keith Runge, S. B. Trickey, and Frank E. Harris*	**Graded Methods for Quantum Mechanical Force Generation in Molecular Dynamics Simulations**
12:45 – 13:15	*T. Toraishi and T. Tsuneda*	**Molecular Property of Protactinium(V) and Uranium(VI) oxocations: A Density Functional Theory Study**
13:15 – 13:45	*T. P. Straatsma*	**Lipopolysaccharide Membranes and Membrane Proteins of *Pseudomonas aeruginosa* Studied by Computer Simulation**

Friday 27 October 2006 SESSION: COMPUTATIONAL METHODS CHAIR: BJØRN KVAMME (ROOM 5)		
15:30 – 16:00	*Tatsuya Hattori, Takashi Toraishi, Takao Tsuneda and Satoru Tanaka*	**Investigations of poor DFT calculations of actinides: Reduction of UO_2^{2+} ion**
16:00 – 16:30	*Francisco Torrens and Gloria Castellano*	**Polarizability Characterization of Zeolitic Brønsted Acidic Sites**
16:30 – 17:00	*T. Verstraelen, D. Van Neck, P. W. Ayers, V. Van Speybroeck and M. Waroquier*	**The Gradient Curves Method: An improved strategy for the derivation of molecular mechanics valence force fields from ab initio data**
Coffee Break		
17.30 – 18:00	*S. D. Zarić, M. Milčić, M. Stević, I. Holclajtner-Antunović, M. B. Hall*	**Fenske-Hall Calculations on Polyoxometalate Anion**
18:00 – 18:30	*László Gránásy, Bjørn Kvamme*	**Phase Field Modelling of Reaction Between Methane Hydrate and Fluid Carbon Dioxide**
18:30 – 19:00	*Bjørn Kvamme, Remi Åsnes*	**Mechanisms for Kinetic Hydrate Inhibitors**
19:00 – 19:30	*Bjørn Kvamme, Tatyana Kuznetsova, Kurt Schmidt*	**Experimental Measurements and Numerical Modelling of Interfacial Tension in Water-Methane Systems**
19:30 – 20:00	*Bjørn Kvamme, Trygve Buanes, Tatyana Kuznetsova*	**Heterogeneous growth of hydrate on the CO2/aqueous solution interface**
20:00 – 20:30	*Tatyana Kuznetsova, Martin Hovland, Håkon Rueslåtten, Bjørn Kvamme, Hans Konrad Johnsen, Gunnar Fladmark*	**Supercritical Outsalting as a Source of Salt Deposition: Combining Molecular Modeling and Reservoir Simulations**
20:30 – 21:00	*M. Alaoui-Lamrani, M. Addou, L. Dghoughi, N. Fellahi, J. C. Bernède, Z. Sofiani, B. Sahraoui, A. El Hichou, J. Ebothé, R. Dounia, M. Regragui*	**Structural morphological and Cathodoluminescent properties of undoped and Erbium doped nanostructured ZnO deposited by Spray Pyrolysis**

Friday 27 October 2006 SESSION: COMPUTATIONAL METHODS CHAIR: L. K. BIENIASZ (ROOM 6)		
16:00 – 16:30	*L. K. Bieniasz*	**Development of an Adaptive Finite-Difference Strategy for the Automatic Simulation of Transient Experiments in Electrochemical Kinetics**
16:30 – 17:00	*G. Christakos and H-L Yu*	**New Results in Computational Porous Media Upscaling**
Coffee Break		
17:30 – 18:00	*L.K. Bieniasz and H. Rabitz*	**A Solution Mapping Technique for the Rapid Computation of Theoretical Cyclic Voltammograms for Experimental Data Analysis in Electrochemical Kinetics**
18:00 – 18:30	*I. Varlamis and S. Bersimis*	**Providing shortcuts to the learning process**
18:30 – 19:00	*T. Singh, K. Bisetty, H. G Kruger*	**A computational study of the mechanism of formation of the Penta-Cyclo Undecane (PCU) Cage Lactam**
19:00 – 19:30	*Smail Bougouffa*	**Numerical Treatment of Coupled Linear Differential Equations**

Friday 27 October 2006 POSTER SESSION	
18:00 – 20:00	**POSTER SESSION** 1. A. Fountoulakis, A. F. Terzis and E. Paspalakis, Effects of fluctuations and decay in an diabatically controlled SQUID qubit

FRIDAY 27 OCTOBER 2006

21:00 – 23:00

WELCOME DRINK

ELECTRON CORRELATION FOR THE WHOLE PERIODIC TABLE

A theoretical chemistry Symposium in honour of Björn O. Roos

Saturday October 28, 2006 (Room 1)

Schedule	Speaker	Title of the contribution
	Chair	*Peter Schwerdtfeger*
09.00 - 09.30	Michael C. Haeven, Emory, Atlanta, USA	*Probing actinide electronic structure using fluorescence and multi-photon ionization spectroscopy*
09.30 - 10.00	Valérie Vallet, Lille, France	*The importance of electron correlation and intermediate coupling in the spectroscopy of actinide molecules*
10.00 - 10.30	Pekka Pyykkö, Helsinki, Finland	*News on heavy-element chemistry*
10.30 - 11.00	**COFFEE BREAK**	
	Chair	*Valera Veryazov*
11.00 - 11.30	Luis Serrano-Andrés, Valencia, Spain	*DNA nucleobases photoreactivity : The role of quantum chemistry in modern photochemistry*
11.30 - 12.00	Christel M. Marian, Düsseldorf, Germany	*Vibronic spin-orbit coupling: a clue to intersystem crossing in psoralen*
12.00 - 12.30	Luis Seijo, Madrid, Spain	*Ab initio calculations on lanthanide and actinide ions in solids using MOLCAS*
LUNCH		
	Chair	*Per-Åke Malmqvist*
15.30 - 16.00	Gernot Frenking, Marburg, Germany	*Multiple bonds in heavy atom molecules : To be or not to be, that is the question*
16.00 - 16.30	Chantal Daniel, Strasbourg, France	*From small organometallics to large metal-to-ligand-charge-transfert complexes : excited states quantum chemistry*
16.30 - 17.00	**COFEE BREAK**	
17.00 - 17.30	Odile Eisenstein, Montpellier, France	*Organometallic reactivity from a computational point of view: some recent examples*
17.30 - 18.00	Michael B. Hall, Texas A&M, Texas, USA	*Modeling metaloenzymes: Nickel-iron and di-iron hydrogenases*
18.00 - 18.30	Jennifer C. Green, Oxford, UK	*Accessing two final states by ionizing the f electron in a Ce(III) compound*
18.30 - 20.30	**Poster Session**	**Jointly together with the Peter Schwerdtfeger symposium**

POSTER SESSION

ELECTRON CORRELATION FOR THE WHOLE PERIODIC TABLE
A theoretical chemistry Symposium in honour of Björn O. Roos

AND

RELATIVISTIC QUANTUM THEORY: COMPUTATIONAL PERSPECTIVES AND APPLICATIONS

Saturday October 28, 2006
18:30 – 20:30

1) N. Gilka, C. M. Marian, P. R. Taylor
Implementation: Electron Spin-Spin-Coupling

2) Juraj Raab, Roland Lindh, Lester Andrews and Laura Gagliardi
Theoretical Study of the U_nH_m species (n=1,2; m=1,2,4,6)

3) Mercedes Rubio, Daniel Roca-Sanjuán, Manuela Merchán, and Luis Serrano-Andrés
Ionization potentials of DNA and RNA components

4) Steven Vancoille
Calculation of EPR g-tensors for transition metal complexes using a sum-over-states based CASSCF/CASPT2/RASSI-LSO method

5) B. Assadollahzadeh1, S. Schäfer, P. Schwerdtfeger
Polarizabilities of medium-sized tin clusters (Sn10-Sn18): A DFT Study

6) S. Biering, A.Hermann, W.G. Schmidt
A Density functional approach to the adsorption of water on chlorine-terminate Si(111)

7) A. Hermann, P. Schwerdtfeger
Magnetic Properties of α_-CrCl2: Benchmarking first principles methods

8) C. Thierfelder and P. Schwerdtfeger
Relativistic effects in superheavy hydrids

9) Dariusz Kędziera
Solving of the infinite-order two-component method equations

International Conference of Computational Methods in Sciences and Engineering 2006 (ICCMSE 2006)

4th Mathematical Chemistry Symposium in honour of Nenad Trinajstic on the occasion of his 70th birthday.

Symposium Organizer: Sonja Nikolic

SATURDAY, 28 OCTOBER 2006 (Room 2)

Oral Presentations

Schedule	Speaker	Title of contribution
Chair: Sonja Nikolic, Zagreb, Croatia		
09:00–09:05	Sonja Nikolic	Opening
09.05 - 09.25	Danail G. Bonchev, Richmond, Virginia, USA	Molecular *vs*. Biological Structure. A Comparative Analysis
09:25 – 09:45	Paul G. Mezey, Newfoundland, Canada	Molecular Graphs as the Essence of All Molecular Models - A Molecular Physics Perspective
09:45 – 10:05	Damir Nadramija, Zagreb, Croatia	Data visualization of multivariate (non)linear regression ensembles in QSAR/QSPR
10:05 – 10:25	Henryk Chojnacki, Wrocław, Poland	Electronic Structure of Some Model Anti Molecular Systems. Possible Role of Relativistic Effects
10:25-10:50	**COFFEE BREAK**	
Chair: Danail G. Bonchev, Richmond, Virginia, USA		
10:50 - 11:10	James Devillers, Rillieux La Pape, France	Modeling the Endocrine Disruption Profile of Xenobiotics
11:10 - 11:30	Carlo Bertinetto, Pisa, Italy	Recent Advances in the Representation of Molecular Structures for RecNN-QSPR Analysis

Continued		
11:30 – 11:50	Sonja Nikolic, Zagreb, Croatia	On Zagreb Matrices and Derived Descriptors
11:50 – 12:10	Igor G. Zenkevich, St. Petersburg, Russia	Application of Recurrent Relationships in Approximation of Physico-Chemical Properties of Any Homologues of Organic Compounds
Chair: Igor G. Zenkevich, St. Petersburg, Russia		
12:10 – 12:30	Peter L. Simon, University Budapest, Hungary	Transverse instability of non-adiabatic flames
12:30 – 12:50	Guillermo Restrepo, Pamplona, Colombia and Bayreuth, Germany	Modelling the fate of alkanes in rivers
12:50 – 13:10	Koh-hei Nitta, Kanazawa, Japan	Graph-Theoretical Approach to Rheological Properties of Branched Gaussion
13:10 – 13:30	Fernando Ruette, Caracas, Venezuela	A quantum parametric method (CATIVIC) implemented for molecular simulation of surface reactions
13:30 – 13:50	Guillermo Restrepo, Pamplona, Colombia and Bayreuth, Germany	Measuring dissimilarity between dendrograms
13:50 – 14:10	Zdenek Slanina, Taipei, Taiwan	Fullerenes and Metallofullerenes: Theoretical Measures of Their Thermodynamic and Kinetic Stabilities
LUNCH		
09:00 – 14:00 **Parallel Poster Session**		
	Ivan Basic, Zagreb, Croatia	Improvement of QSAR of flavonoids by using autocorrelation functions weighted by different atomic properties
	Lech Schultz, Poznan, Poland	Electron Density Distribution and Self-Assemblage Symmetries of Molecular Systems - a Fuzzy-Set Based Assessment

Saturday 28 October 2006

SESSION: COMPUTATIONAL METHODS AND MODELLING
CHAIR:
D.S. VLACHOS (ROOM 2)

15:30 – 16:00	*J. M. Matías, J. C. Reboredo, T. Rivas*	**Forecasting the direction of stock return movements using Bayesian networks**
16:00 – 16:30	*S. Hwang, and J. Jang*	**Molecular Dynamics of Thin-Film Formation in Dip-Pen Nanolithography**
16:30 – 17:00	*Giovanni Cavaccini, Vittoria Pianese, Alessandra Jannelli, Salvatore Iacono, and Riccardo Fazio*	**Mathematical and Numerical Modeling of Liquids Dynamics in a Horizontal Capillary**
17:00 – 17:30	*Abel J. P. Gomes and José F. M. Morgado*	**Numerical computation of isolated points for implicit curves and surfaces**
Coffee Break		
18:00 – 18:30	*L. S. Iliadis, S. I.Spartalis, A. Paschalidou*	**Neural Modeling of the Tropospherical Ozone Concentration**
18.30 – 19:00	*M. Pezzotta and Z. L. Zhang*	**Cohesive Zone Modeling of Grain Boundary Micro-cracking in Ceramics**
19:00 – 19:30	*Tae Yong Kim and HoonJae Lee*	**TM Wave Propagation Simulation using Java Multithreading for Domain Decomposition Approach**
19:30 – 20:00	*Hoon Ko, Hongil Kim*	**A Study on Group Key Management Model in Wire/Wireless Distribute Group Environments**
20:00 – 20:30	*P. Kyriazis, C. Anastasiadis, D. Triantis and J. Stonham*	**Wavelet analysis of ac conductivity time series for the detection of imperfections in rocks**
20:30 – 21:00	*J. M. Matías, T. Rivas, J. Taboada and C. Ordóñez*	**Construction of an expert system for the evaluation of slate quality using machine learning techniques**

Low-dimensional Semiconductor systems

Saturday October 28, 2006 (Room 3)

Schedule	Speaker	Title of contribution
09:00-09:10	A. D. Zdetsis	***OPENING***
	Chair	R. Magri
09:10-09:40	A.N. Andriotis, R. M. Sheetz and M. Menon	*Defect induced magnetism in C_{60} and Single-Wall Carbon Nanotubes: The role of vacancies and impurity atoms*
09:40-10:00	A. Mavrandonakis G. Mpourmpakis, G. E Froudakis	*SiCNTs: a novel material for tips and storage applications*
10:00-10:20	E. N. Koukaras, C. S. Garoufalis and A. D. Zdetsis	*Ab initio study of optical and electronic properties of silicon and germanium nanowires*
10:20-10:40	C. S. Garoufalis	*A TDDFT analysis of the polarizabilities of small Si_n(n=3-6) clusters through their excitation energies and oscillator strengths*
10:40-11:10	A. D. Zdetsis	*Metal encapsulated silicon clusters*
11:10-11:40		**COFFEE BREAK**
	Chair	A. N. Andriotis
11:40-12:10	C. V. Ciobanu	*Global Optimization of 1- and 2-Dimensional Nanoscale Structures*
12:10-12:30	R. Magri, E. Degoli, F. Iori, O. Pulci, S. Ossicini,G. Cantele, F. Trani, D. Ninno	*Role of surface passivation and doping in Silicon Nanocrystals*
12:30-12:50	A.S. Moskalenko and J. Berakdar, A.A. Prokofiev and I.N. Yassievich	*Multiband effective mass theory for Si quantum dots*
12:50:13:10	M. Springborg	*Elecdtronic properties of Semiconductor Nanoparticles*
13:10-13:30	E. Paspalakis, M. Tsaousidou, A. Kanaki and A. F. Terzis	*Conditions for high-efficiency population transfer in a semiconductor quantum well structure*
LUNCH		
18:00-19:00		**POSTER SESSION**
	E. N. Koukaras, C. S. Garoufalis and A. D. Zdetsis	*Ab initio study of electronic and structural properties of $Ni@Si_{10}$ cluster*
	A. D. Zdetsis, E. N. Koukaras and C. S. Garoufalis	*A Comparative DFT and MPn study of isoelectronic $[Co@Si12]^{-1}$, $[Ni@Si_{12}]$ and $[Cu@Si_{12}]^{+1}$*

"Computational Electronics: Physical Modeling, Mathematical Theory, and Numerical Algorithm"

Saturday 28 October, 2006 (Room 3)

Schedule	Speaker	Paper title
Chair: Prof. Yiming Li		
15:00-15:30	Yiming Li	Electron Energy State Spin Splitting in Nanoscale InAs/GaAs Semiconductor Quantum Rings
15:30:-15:50	Lynda Cherfi	A new Riccati type algorithm for coupled algebraic MCV Riccati equations
15:50-16:10	Yu-Kuang Chen	An Improved Efficiency of the Frank-Wolfe Algorithm for Network Traffic Assignment
16:10-16:30	Chien-Lun Lan	Parallel Chain Convergence of Time Dependent Origin-Destination Matrices with Gibbs Sampler
16:30-17:00	**Coffee Break**	
Chair: Prof. Yiming Li		
17:00-17:20	Shao-Ming Yu	A Unified Optimization Framework for Real World Problems
17:20-17:40	Ntalaperas Dimitrios	Simulation of the Single Qubit Phase Operation in an Ionized P_2 Donor Molecule Implanted on S_i Semiconductor Material
17:40-18:00	Chien-Lun Lan	Statistical Estimation of Dynamic Tobit Models
18:00-18:20	Yi-Shan Li	The Prevalence of Paradox in Transportation Network Design Problem

“Computational Methods in Molecular Biology: Theory and Applications”

Saturday October 28, 2006 (Room 4)
Chairmen: Athanasios Tsakalidis, Christos Makris

Schedule	Speaker	Title of Contribution
10:00-10:20	E. Theodoridis, University of Patras	Implementation of Efficient Data Structures for Statistical Processing of Proteins
10:25-10:45	A.Bakalis, Department of Computer Science, King's College, England	Algorithms for Bitmasking Strings.
10:50-11:10	E. Theodoridis, University of Patras	A parallel system architecture for biology and medical concept discovery from biological corpora.
11:15-11:35	L. Skarlas, University of Patras	MAPS: MicroArray Processing Software for management, data mining and visualization of gene expression data.
11:40-12:00	G. Sotiropoulou, University of Patras	Computational Cloning and Analysis of Human Kallikrein and Orthogonal Genes

Vedene Smith Memorial Symposium, Crete, 2006
Oct. 28–30

Saturday October 28, 2006 (Room 4). Session 1. Chair: A.J. Thakkar		
12:15–12:30	A. J. Thakkar	The life and work of Vedene H. Smith, Jr.
12:30–13:00	A. D. Becke	Post-Hartree-Fock correlation models.
13:00–13:30	W. Kutzelnigg	Density cumulant functional theory.
13:30–14:00	M. DeFranceschi	An epitome of quantum chemistry in momentum space.
14:00–15:30	**Lunch break**	
15:30–16:00	R. J. Bartlett	Coupled-cluster theory for large molecules: The natural linear scaled coupled-cluster method.
16:00–16:30	F. E. Harris	Current studies of few-electron systems.
16:30–17:00	M. Klobukowski	Effects of quantum confinement on molecular structure, spectra, and reactivity.
17:00–17:30	**Coffee break**	
Saturday October 28, 2006 (Room 4). Session 2. Chair: E.R. Davidson		
17:30–18:00	E. R. Davidson	Charge and spin distributions.
18:00–18:30	P. G. Mezey	Size measures of molecular electron densities — From the Smith measure of electron pairs to local and global macromolecular measures.
18:30–19:00	I. P. Hamilton	Quantum-classical correspondence for the kinetic energy.
19:00–19:30	**Coffee break**	
19:30–20:00	P. Ziesche	The electron-gas pair density and its geminal description.
20:00–20:30	W. Weyrich	An electronic position and momentum density study of chemical bonding in TiO_2 (Rutile).
20:30–21:00	P. Becker	Density matrices, the central link between observations and theory.
October 28, 2006. Poster Session		
18:30–20:30	T. Tsukamoto	Electronic properties of solvated duplex DNAs by DFT calculations

3rd Symposium on "Industrial and Environmental Case Studies"

Symposium Organizer: Fragiskos A. Batzias

Saturday, 28 October 2006 (Room 5)

Oral Presentations

Schedule	Author(s)	Title of contribution
11.25-11.30	F.A. Batzias	Opening and Chair
11.30-11.45	Hatzigiannakis, G.K. Arampatzis, A.G. Panoras, and A.K. Ilias	Soil monitoring in Halastra - Kalohori area
11.45-12.00	N.K. Lazaridis,, G.Z. Kyzas, A.A. Vassiliou, D.N. Bikiaris	Dye removal from aqueous solutions by sorption onto chitosan derivatives
12.00-12.15	E. H E. Hatzigiannakis, E. Anastasiadou – Partheniou	Finite differences model for simulation of flood wave propagation in a Pinios river section
12.15-12.30	I. Chatzispiroglou, E. Anastasiadou-Partheniou , T. Zissis	Effect of Pinios riverbed parameters to flood wave propagation
12.30-12.45	J.L. Díez, J.M. Gozálvez-Zafrilla, F. Barceló, A. Santafé-Moros	Velocity-based fuzzy local modelling and control of continuous distillation towers
12.45-13.00	F.A. Batzias	Multicriteria Choice of Enzyme Immobilization Process for Biosensor Design and Construction
13.00-13.15	M. Valyrakis , P. Diplas, C. L. Dancey	Short time prediction of chaotic time series using ANFIS
13.15-13.30	S.I. Yannopoulos , S.Basbas, I.S. Giannopoulou	Management of Water Bodies Pollution due to the Interurban Roads Stormwater Runoff
Lunch		
14.55-15.00	G. Lagioia	Opening and Chair
15.00-15.15	G. Lagioia , V. Amicarelli, O. De Marco	On the utility of combining two analytical methodologies: Material Flow Analysis (MFA) and Input Output Accounting (IOA)

15.15-15.30	P. Fotilas, F.A. Batzias	Endogenous Determination of Dimensionless Energy Indices for Industrial Management
15.30-15.45	I.V. Yentekakis , G. Goula, T. Papadam	A Novel Biogas-Fueled-SOFC Aided Process for Direct Production of Electricity from Wastewater Treatment: Comparison of the Performances of High and Intermediate Temperature SOFCs
15.45-16.00	G. P. Giatrakos, P. G. Mouchtaropoulos, G. D. Naxakis, T. D. Tsoutsos	Energy Planning of a Hydrogen - SAPS System Using Renewable Sources for Karpathos Island, Greece
16.00-16.15	H.E. Keenan , P.Sentenac, A. Songsasen, A. Sakultantimetha, S. Bangkedphol	Monitoring and Modeling of metals and PAH contaminants in Thai: Laos Mekong River
16.15-16.30	M. Pislaru , A. Trandabăț	Fuzzy model for environmental sustainability assurance
Coffee Break		
17.00-17.15	B. Bilitewski, M. Schirmer	Waste to Energy
17.15-17.30	C. Martín-Sistac, G. Escudero and M. Graells	Efficient Management of Wastewater Treatment Networks
17.30-17.45	D.E. Koulouriotis and D.M. Emiris	An Intelligent Decision Support System for Industrial Robot Selection
17.45-18.00	F.A. Batzias and C. Saridaki	On the Determinants of Optimal Capacity of Water Treatment Plants Operating within a Network
18.00-18.15	G. Martinopoulos , G. Tsilingiridis and N. Kyriakis	Life Cycle Analysis Implementation for CO_2 Abatement in Energy Systems – The Case of Solar Thermal Systems
18.15-18.30	E. Mousoulis, E. Dimitriou	Hydrological modelling in trichonis lake catchment and the respective impacts from land use changes during the last 50 years

Saturday, 28 October 2006
Parallel Poster Session

Schedule	Author(s)	Title of contribution
11.30-18.30	F.A. Batzias	Decreasing the Cost of Industrial Processes through Chemical Kinetics
	D.M. Emiris and D.E. Koulouriotis	A Systematic Approach to the Grammar and Syntax of Assembly Rules for the Flexible Development of Composite Production Systems
	D.F. Batzias	The Influence of Oil-Price-Dependent Macroeconomic Variables/Parameters on Subsidies for Promoting Renewable Energy Supply
	Glytsos T., Smolík J. and Lazaridis M.	Characterization of Indoor Air Quality Using an Indoor/Outdoor Microenvironmental Model

LINEAR AND NON LINEAR OPTICAL PROPERTIES
A Theoretical Chemistry Symposium dedicated to Professor A. D. Buckingham

Saturday October 28, 2006 (Room 6)

Schedule	Speaker	Title of contribution
9:00 – 9:10	M. G. Papadopoulos, Athens, Greece	*Opening and chair*
9:10-9:40	T. Saue, Strasbourg,France	*4-component relativistic molecular response calculations*
9:40-10:10	F.L.Gu, Fukuoka, Japan	*Elongation Coupled-Perturbed Hartree-Fock Method*
10:10-10:40	P. Calaminici, Cinvestav, Mexico	*Transition metal clusters polarizabilities*
10.30 – 11.00	**COFFEE BREAK**	
	Chair: H. Reis	
11.00 – 11.30	M. G. Papadopoulos, Athens, Greece	*A systematic study of the linear and non-linear optical properties of small molecules and clusters: The correlation, vibrational and relativistic contributions*
11.30 – 12.00	W. Bartkowiak, Wrocław, Poland	*Solvatochromism and Two-Photon Absorption of Donor-Acceptor Organic Chromophores*
12:30-13:15	P. C. Ray, Mississippi, USA	*Nonlinear Optical Properties of Molecular Aggregates: From Push-Pull Organic Chromophores to DNA coated Gold Nanoparticles*
13:15-15:00	**LUNCH BREAK**	
	Chair: A. Avramopoulos	
15:00-15:30	S. Tretiak, Los Alamos NM, USA	*Nonlinear optical response and photodynamics of conjugated molecules: effects of branching and substitution*
15:30-16:00	A. Mayer, Namur, Begium	*A charge-dipole model to compute the polarizability of fullerenes and carbon nanotubes.*
16:00-16:30	S. Ramasesha, Bangalore, India	*Computation of Linear and Nonlinear Optical Response and Real Time Dynamics of Intermolecular Electronic Processes in Correlated Molecular Electronic Systems.*
16:30-17:00	**COFFEE BREAK**	
	Chair: W. Bartkowiak	
17:30-18:00	S. Coriani	*On the Buckingham birefringence in atoms and molecules*

SATURDAY 28 OCTOBER 2006

22:00 – 23:30

CONFERENCE CONCERT
(for the program, please see at the end of the ICCMSE 2006 Program)

ELECTRON CORRELATION FOR THE WHOLE PERIODIC TABLE

A theoretical chemistry Symposium in honour of Björn O. Roos

Sunday October 29, 2006 (Room 1)

Schedule	Speaker	Title of the contribution
	Chair	*Manthos Papadopoulos*
09.00 - 09.30	Cristina Puzzarini, Bologna, Italy	*How accurately can structural, spectroscopic and thermochemical properties be predicted by ab initio computations?*
09.30 - 10.00	Tomasz Wesolowski, Geneva, Switzerland	*Eliminating orbitals from quantum mechanical description of many-electron systems : A step beyond Kohn-Sham*
10.00 - 10.30	Jun-ya Hasegawa, Kyoto, Japan	*Photobiology and biospectroscopy studied by SAC-CI method*
10.30 - 11.00	**COFFEE BREAK**	
	Chair	*George Froudakis*
11.00 - 11.30	Antonio Rizzo, Pisa, Italy	*Non linear optical properties of chiral molecules*
11.30 - 12.00	Jeppe Olsen, Aarhus, Denmark	*Bridging the gap between multi-reference perturbation and coupled cluster methods*
12.00 - 12.30	Henry F. III Schaefer, Athens, USA	*Lesions in DNA subunits: Foundational studies of structures and energetics*
12.30 - 12.40	Henry F. III Schaefer, Athens, USA	*Concluding remarks*
LUNCH		

Sunday 29 October 2006 SESSION: COMPUTATIONAL AND NUMERICAL METHODS (INVITED SPEAKERS) CHAIR: D.S. VLACHOS (ROOM 2)		
09:30 – 10:30	*N.S. Scott, L.Gr. Ixaru, C. Denis, F. Jézéquel, J.-M. Chesneaux and M.P. Scott*	**High performance computation and numerical validation of e-collision software**
10:30 – 11:30	*H.J. Herrmann, O. Durán and E.J.R. Parteli*	**Modelling dunes with vegetation and dunes on Mars**
11:30 – 12:30	*L. Gr. Ixaru*	**Lagrange-like error formula in exponential fitting**

SUNDAY 29 OCTOBER 2006

13:00

EXCURSION(For more information on Conference Site)

SUNDAY 29 OCTOBER 2006

20:00

CENTRAL DINNER(For more information on Conference Site)

Relativistic quantum theory: Computational perspectives and applications.

Crete, October 30 - November 1 2006

Programme

Poster Session jointly together with the Roos Symposium : October 28, 18.30 to 20.30

Monday October 30, 2006 (Room 1)

Schedule	Speaker	Title of contribution
09.00 - 09.10	Peter Schwerdtfeger (Auckland, New Zealand)	*OPENING and CHAIR*
09.10 - 09.50	Ian Grant (Oxford, UK)	*The Beauty of Spinors.*
09.50 - 10.20	Timo Fleig (Düsseldorf, Germany)	*A 4-Component General-Order Multi-Reference Coupled Cluster Method. Development and Initial Application.*
10.20 - 10.50	Haruyuki Nakano (Fukuoka, Japan)	*Multireference perturbation theory with four-component general multiconfigurational reference functions.*
10.50 - 11.10	**COFFEE BREAK**	
	CHAIR : Trond Saue	
11.10 - 11.40	Miroslav Urban (Bratislava, Slovakia)	*Relativistic and electron correlation effects as a tool for explaining some trends in molecular properties and interactions*
11.40 - 12.10	Josef Anton (Kassel, Germany)	*Relativistic Density Functional Theory.*
12.10 - 12.40	Leonardo Belpassi (Perugia, Italy)	*Computational strategies based on electron density fitting in relativistic 4-component density functional theory.*
12.40 - 13.10	Luuk Visscher (Amsterdam, Netherlands)	*Relativistic methods for relatively small systems.*
LUNCH		

Monday October 30, 2006 (Room 1) – Continued		
	CHAIR : Beate Paulus	
15.00 - 15.30	Hermann Stoll (Stuttgart, Germany)	*On the accuracy of small-core and large-core pseudopotentials.*
15.30 - 16.00	Ivan Lim (KAIST, Korea)	*On the Properties of Alkaline-earth Dihydrides: Relativistic Consideration.*
16.00 - 16.30	Matthias Lein (Auckland, New Zealand)	*Relativistic pseudopotential calculations for catalytic reactions of Au(III).*
17.00 - 17.30	**COFFEE BREAK**	
	CHAIR : Luuk Visscher	
17.30 - 18.00	Markus Reiher (Zürich, Germany)	*On the calculation of properties in the Douglas-Kroll-Hess framework.*
18.00 - 18.30	Alexei Matveev (München, Germany)	*Methods in heavy element chemistry - Linear response in DKH.*
18.30 - 19.00	Marco Tomaselli (Darmstadt, Germany)	*Relativistic Time Dependent Model for n-Electrons Systems in Strong Laser Fields.*
19.00 - 19.30	Yasuyuki Ishikawa (San Juan, Puerto Rico)	*Relativistic R-matrix based on relativistic MR-MBPT description of atomic target.*

Computational Spectroscopy

Organizers:

B.Champagne, U.Hohm, G. Maroulis and C.Pouchan

Monday October 30, 2006 (Room 2)

Schedule	Speaker	Title of contribution
	Chair: C.Pouchan	
9:00 – 9:40	W.Glaz	Collisional ab initio hyperpolarizabilities in computing hyper-Rayleigh spectra of noble gas heterodiatomics
9:40-10:10	U.Hohm	Problems in the experimental determination of higher-order dipole-polarizabilities
10:10-10:40	D.Begué	Influence of impurities and by-products in the vibrational spectra of reactive compounds
10.40 – 11.00	**COFFEE BREAK**	
	Chair: B.Champagne	
11:00–11:40	Mihaeng Cho	Coherent Two-Dimensional Optical Spectroscopy
11:40 – 12:10	S.Farantos	Periodic Orbits in Biological Molecules: Phase Space Structures and Selectivity
12:10-12:50	M.C. Ruiz Delgado	Perfluorination of Tetracene: Raman Study and Charge Transport Properties Aided by Quantum-Chemical Calculations
12:50-13:10	C.Lapouge	Quantum Chemical Simulation of Resonance Raman and UV-visible Spectra
13:10-15:00	**LUNCH BREAK**	
	Chair: **U.Hohm**	
15:00-15:40	B.M.Rode	Ab initio Quantum Mechanical Charge Field (QMCF) Simulations: New Horizons in Solution Chemistry
15:40-16:10	C.Pouchan+P.Carbonière	Anharmonic calculation of vibrational spectra for P_4O_6 and P_4O_{10} systems.
16:10-16:40	C.Iung	Theoretical study of specific, highly excited states in DFCO
16:40-17:00	**COFFEE BREAK**	
	Chair: **B.M.Rode**	
17:00-17:40	K.Szalewicz	Spectra of water dimer from ab initio calculations
17:40-18:10	A.Laganá	Towards the Grid design of the dynamics engine of a molecular simulator
18:10-18:30	R.Prosmiti	Theoretical simulation of the sequential photodissociation dynamics of the HI dimer
18:30-19:00	P.Karamanis	Does second order møller-plesset perturbation theory predict the correct equilibrium geometry for Si_6? a critical analysis of current investigations.

Computational Quantum Chemistry: applications from the atomic to the nanoscale

Organizer: **George Maroulis**

Monday October 30, 2006 (Room 3)

Schedule	Speaker	Title of contribution
	Chair: G.Maroulis	
9.00 – 9.40	K.Yamaguchi	General spin orbital density functional study of transition metal clusters and complexes
9.40-10.20	M.Urban	Optimized virtual orbital space (OVOS) as a tool for more efficient correlated and relativistic calculations of molecular properties and interactions
10.20-10.40	B.Randolph	Computer Systems for Quantum Mechanical Simulations
10.40 – 11.00	**COFFEE BREAK**	
	Chair: M.Nakano	
11.00 – 11.40	J.Leszczynski	Guanine. Structures, Properties and Interactions – From the Isolated Ground State to Excited States in Polar Solvent
11.40 – 12.20	S.Canuto	Molecular Polarization in Liquid Environment
12.20-13.00	S.Zalis	The Modeling of the Interaction of Organic Molecules with Gold and Platinum Clusters
13.00-13.20	H.-M.E	Approximate String Matching Based on Bit Operations
13.15-15.00	**LUNCH BREAK**	
	Chair: **M.Urban**	
15.00-15.40	I.Kaplan	Problems in the Density Functional Method with the Total Spin and Space degeneracy
15.40-16.20	K.Hirao	A new hybrid DFT functional - Accurate description of response properties and van der Waals interactions
16.20-16.40	T.S.Hofer	The hydration structure of Pd(II) in aqueous solution obtained from a QMCF MD simulation
16.40-17.00	**COFFEE BREAK**	
	Chair: **J.Leszczynski**	
17.00-17.40	J.Jellinek	**Site-Specific Polarizabilities. Probing the Atomic Response of Silicon Clusters to an External Electric Field**
17.40-18.20	C.Cramer	SMx Continuum Models for Condensed Phases
18.20-19.00	Joachim Sauer	Structure and Reactivity of Metal Oxides: Small Gas Phase Species, Nanoclusters, Solid Catalysts
19.00-19.20	I. Kratochvilova	Electronic structure calculations on Molecular Photo-FET

Poster Session Monday 30/10/2006 19:30 – 21:30:

C.Koukounas, S.Kardahakis, E.Miliordos, C.Bae

COMPUTATIONAL APPROACHES TO SUPRAMOLECULAR CHEMISTRY

Monday October 30 2006 (Room 4)

Schedule	Speaker	Title of contribution
8:00 – 9:10	Jin Yong Lee, Suwon, Korea	*OPENING*
	Chairperson	*Prof. Manabu Sugimoto*
9:10 – 9:40	Prof. Pekka Pyyko, Helsinki, Finland	*The metallophilic attraction: Theory*
9:40 – 10:10	Prof. Jun-ya Hasegawa, Kyoto, Japan	*Excited States and Electron-transfer in Bacterial Photosynthetic Reaction Center: SAC-CI Theoretical Study*
10:10 – 10:30	**COFFEE BREAK**	
	Chairperson	*Prof. Cheol Ho Choi*
10:30 – 11:00	Prof. Helena Dodziuk, Warsaw, Poland	*Modeling of molecular and chiral recognition by cyclodextrins*
11:00 – 11:30	Prof. Jin Yong Lee, Suwon, Korea	*Computational approaches to Molecular Functions*
11:30 – 12:00	Prof. GuanHua Chen, Hong Kong, China	*Existence of A Density-Functional Theory for Open Electronic System*
LUNCH		
	Chairperson	*Prof. Helena Dodziuk*
2:00 – 2:30	Dr. Hirotoshi Mori, Fukuoka, Japan	*Computational Design of Proton-Electron Coupling System for Optically Durable Molecular Memory*
2:30 – 3:00	Prof. Serguei Fomine, Mexico, Mexico	*Oligothiophene catenanes and Knots: A DFT Study*
3:00 – 3:30	Prof. Jun Hyung Cho, Seoul, Korea	*Theoretical Prediction of Heterogeneous Molecular Wires on the Si(001) Surface*

Continued

COMPUTATIONAL APPROACHES TO SUPRAMOLECULAR CHEMISTRY

Monday October 30 2006 (Room 4)

	Chairperson	*Prof. GuanHua Chen*
3:30 – 4:00	Prof. Sukmin Jeong, Jeonju, Korea	*Adsorption of organic molecules on a high-index Si surface*
4:00 – 4:30	Prof. Cheol Ho Choi, Daegu, Korea	*Theoretical Study of Cycloaddition Reactions of C_{60} on the Si(100)-2x1 surface*
4:30 – 5:00	Dr. Norio Yoshida, Okazaki, Japan	*Selective ion binding by human lysozyme studied by the statistical mechanical integral equation theory*
5:00 – 5:30	**COFFEE BREAK**	
	Chairperson	*Prof. Jin Yong Lee*
5:30 – 6:00	Prof. Chantal Daniel, Strasbourg, France	*Molecular switch effect in Ru(II) complexes intercalated in DNA: a theoretical study*
6:00 – 6:30	Prof. Manabu Sugimoto, Kumamoto, Japan	*Computational Analyses on Electronic Supramolecular Functions. Environment Dependence and Molecular Recognition*
6:30 – 6:40	Prof. Manabu Sugimoto, Kumamoto, Japan	*CLOSING*

LINEAR AND NON LINEAR OPTICAL PROPERTIES
A Theoretical Chemistry Symposium dedicated to Professor A. D. Buckingham (Continued)

Monday October 30, 2006 (Room 5)

Schedule	Speaker	Title of contribution
	Chair: R. Cammi	
9:00 – 9.30	H. Sekino, Tenpaku-cho Toyohashi, Japan	*Evaluation of Polarizability by Density Based Methods*
9:30-10:00	D. N. Beratan, Durham, NC ,USA	*Designing Molecules by Optimizing Potential.*
10:00- 10:30	M. Springborg, Saarbrücken, Germany	*Infinite, periodic systems in external fields*
10.30 – 11.00	**COFFEE BREAK**	
	Chair: H. Sekino	
11.00 – 11.30	R.W. Góra, Wrocław, Poland	*On the influence of intermolecular interactions on the electric properties of molecular aggregates*
11:30 – 12:00	M. Guillaume, Namur, Belgium	*Determination of the Linear and Nonlinear Susceptibilities of Polyacetylene Fibers and Silicon Clusters using Electrostatic Interaction Schemes*
12:00– 12:30	P.-O. Åstrand, Trondheim, Norway	*Molecular mechanics model for electronic polarization: A combined atom-atom charge-transfer and point-dipole interaction model*
12:30-13:15	T. la Cour Jansen, Groningen, Netherlands	*Simulation of two-dimensional infrared spectra by numerical integration of the Schrödinger equation*
13:15-15:00	**LUNCH BREAK**	
	Chair: M. Guillaume	
15:00-15:30	Kurt V. Mikkelsen, Copenhagen, Denmark	*Two-photon absorption cross sections: An investigation of structural environmental effects.*
15:30-16:00	Brian Space, Tampa, FL, USA	*Time Correlation Theories of Nonlinear Spectroscopy*
16:00-16:30	R. Cammi, Parma, Italy	*A short history of the Polarizable Continuum Model methodology for the calculation on linear and nonlinear optical properties of molecules in solution.*
16:30-17:00	**COFFEE BREAK**	

	Chair: P. –O. Åstrand	
17:00-17:30	A. Avramopoulos, Athens, Greece	*A study of the environmental effects on the microscopic and macroscopic non-linear optical properties of liquids, based on a multipolar approximation: Liquid acetonitrile.*
17:30-18:00	B.M. Ladanyi, Colorado, USA	*Polarizability anisotropy dynamics in one and two-component aromatic liquids*
18:00-18:30	H. Reis, Athens, Greece	*Recent advances in the computation of linear and nonlinear optical susceptibilities of polymers, liquids, solutions and crystals using discrete local field theory*

Vedene Smith Memorial Symposium, Crete, 2006
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Monday October 30, 2006 (Room 6). Session 3. Chair: D. Salahub		
09:00–09:30	D. Salahub	Towards the QM/MM modeling of complex biosystems with density functional theory and other tools.
09:30–10:00	S. Larsson	Understanding superconductivity.
10:00–10:30	P. Petelenz	Theoretical models for electroabsorption spectroscopy of organic molecular crystals.
10:30–11:00	**Coffee break**	
11:00–11:30	R. J. Woods	Incorporating charge polarization in classical force fields.
11:30–12:00	R. E. Brown	Influence of metal cations on the intramolecular hydrogen-bonding network and pKa in phosphorylated compounds.

SYMPOSIUM: ADVANCES IN HYDROGEN BOND RESEARCH

Monday October 30, 2006 (Room 6)

Schedule	Speaker	Title of contribution
12.15 – 12.30	Marek Wójcik (Krakow, Poland)	OPENING and CHAIR
12.30 – 13.00	Branka Ladanyi (Fort Collins, USA)	*Computer simulation of polarizability anisotropy dynamics in water-formamide mixtures*
13.00 – 13.30	Janez Mavri (Ljubljana, Slovenia)	*Simulation of tunneling in enzyme catalysis : application to lipoxygenase*
13.30 – 14.00	Hiroshi Sekiya (Fukuoka, Japan)	*Mechanism of multiple-proton transfer in hydrogen-bonded clusters in the gas phase*
14.00 – 15.30	**LUNCH BREAK**	
	CHAIR: Branka Ladanyi	
15.30 – 16.00	Marek Wójcik (Kraków, Poland)	*Dynamics of protons in hydrogen bonds studied by theoretical methods and vibrational spectroscopy*
16.00 – 16.30	Najeh Rekik (Monastir, Tunisia)	*Theoretical modeling of infrared spectra of cyclic acetylsalicylic acid dimer and its deuterated derivative*
16.30 – 17.00	**COFFEE BREAK**	
	CHAIR: Janez Mavri	
17.00 – 17.30	Stanislas Pommeret (Saclay, France)	*Relation between frequency and H bond length in heavy water*
17.30 – 18.00	Masanori Tachikawa (Yokohama, Japan)	*Isotope effect on hydrogen bonds in charged cluster complexes by path integral molecular dynamics method*
18.00 – 18.30	Najeh Rekik (Monastir, Tunisia)	*Infrared spectral density of medium strength H-bonds with the strong anharmonic coupling theory. Both intrinsic anharmonicity of the fast mode and the H-bond bridge. Part II: Isotopic effect*
	CHAIR: Grzegorz Schroeder	
18.30 – 19.00	Piotr Przybylski (Poznan, Poland)	*Spectroscopic, VPO and PM5 semiempirical studies of proton channel formed by methyl ester of monensin A*
19.00 – 19.30	Marek Wójcik (Krakow, Poland)	*Theoretical modeling of the N-H and N-D stretching bands of hydrogen-bonded 1-methylthymine crystal and its deuterated form*

Monday 30 October 2006	
SESSION: HIGHLIGHT LECTURES I **CHAIR: GEORGE MAROULIS (ROOM 1)**	
20:00 – 21:00	**A.D. Buckingham, University of Cambridge, UK**
21:00 – 22:00	**Björn O. Roos, University of Lund, Sweden**

Monday 30 October 2006

POSTER SESSION

21.00-23.00	**POSTER SESSION** 1. Aiko Hayashi, Yokohama-city University, Yokohama, Japan, H/D isotope effect on the lithium bonded cluster by ab initio path integral molecular dynamics simulation 2. Piotr Przybylski and B. Brzezinski, A. Mickiewicz University, Poznan, Poland, AM1d, PM3 as well as PM5 semiempirical studies of Monensin A complexes with monovalent cations and Monensin A hydrates 3. R. Pankiewicz, G. Schroeder and B. Brzezinski, A. Mickiewicz University, Poznan, Poland, Formation of complexes between some lasalocid esters and the monovalent cations studied by spectroscopic and the PM5 semiempirical methods 4. B. Łęska, R. Pankiewicz and G. Schroeder, A. Mickiewicz University, Poznan, Poland, Structures of B- podand's complexes with cations calculated by PM5 semiempirical method 5. S. Bitama, R. Masmoudi, L. Messadia, A. Ferhati, Université de Batna, Algeria, and H. Saadi, Université de M'sila Algeria, Protonation sites of the two-substituted-4,6-di-(alkylamino)-1,3,5-triazines (s-triazines)-interaction with biological unit 6. Young-Won Chang, Myoung-Hee Lee, Cheol-Jung Yoo, Ok-Bae Chang Workflow Mining Based on Heuristic Approach Using Log Data 7. Myoung-Hee Lee , Dae-Gon Kim, Cheol-Jung Yoo, Ok-Bae Chang P2P Business Process Modeling and Implementation Based on Service-Oriented Architecture 8. Gergely Tóth, A Computational Method for Structure Based Hit and Lead Development of Small Molecule Ligands: Modeling Active b-secretase Inhibitors 9. K. C. Ro, S. W. Ko, J. S. Roh, H. S. Ryou , S. H. Lee, A Numerical Study on a Spray System Optimization for Size Reduction of a Wet Type Scrubber 10. Young Hee Park, Kiyull Yang, Yun Hi Kim and Soon Ki Kwon, Ab initio Studies on Acene Tetramers : Herringbone Structure

Relativistic quantum theory: Computational perspectives and applications.

Crete, October 30 - November 1 2006

Tuesday October 31, 2006 (Room 1)

Schedule	Speaker	Title of contribution
	CHAIR : Hermann Stoll	
09.00 - 09.40	Beate Paulus (Dresden, Germany)	*An incremental Method for the Calculation of the Electron Correlation Energy in Metals.*
09.40 - 10.10	Nicola Gaston (Dresden, Germany)	*Ab-Initio Correlation Calculations for the Lattice Structures of Zn, Cd and Hg.*
10.10 - 10.40	Tilo Söhnel (Auckland, New Zealand)	*Changes in Solid State Symmetry due to Relativistic Effects.*
10.40 - 11.00	**COFFEE BREAK**	
	CHAIR : Ian Grant	
11.00 - 11.40	Pekka Pyykkö (Helsinki, Finland)	*QED and the valenve shell.*
11.40 - 12.10	Trond Saue (Strasbourg, France)	*On the variational inclusion of vacuum polarization in 4-component relativistic molecular calculations*
12.10 - 12.40	Uzi Kaldor (Tel Aviv, Israel)	*Towards meV accuracy in atomic spectroscopy calculations: intermediate Hamiltonian relativistic coupled cluster methods with applications to superheavy elements.*
12.40 - 13.10	Ephraim Eliav (Tel Aviv, Israel)	*New formulations of relativistic multireference coupled cluster approach.*
LUNCH		
	CHAIR : Kimihiko Hirao	
15.00 - 15.40	Matthias Schädel (Darmstadt, Germany)	*Superheavy Element Chemistry - Achievements and Perspectives.*
15.40 - 16.10	Burkhard Fricke (Kassel, Germany)	*Applications of full relativistic molecular calculations in the area of superheavy elements.*
16.10 - 16.40	Valeria Pershina (Darmstadt, Germany)	*Theoretical predictions of experimental behaviour of the superheavy elements and relativistic effects.*

Tuesday October 31, 2006 (Room 1) – Continued		
16.40 - 17.00	**COFFEE BREAK**	
	CHAIR : Burkhard Fricke	
17.00 - 17.30	Laura Gagliardi (Geneva, Switzerland)	*Multiple bonds in diactinide compounds.*
17.30 - 18.00	Yuichiro Nagame (Tokai-Mura, Japan)	*Aqueous chemistry of superheavy element, rutherfordium (Rf).*
18.00 - 18.30	Sven Krüger (München, Germany)	*Relativistic density functional studies on actinyl complexation in aqueous solution.*
18.30 - 19.00	Florent Réal (Lille, France)	*Spectroscopy and photochemistry of the uranyl(VI).*
	CHAIR : Pekka Pyykkö	
19.15 - 20.00	***Special Evening Lecture:*** Victor Flambaum (Sydney, Australia)	*Variation of fundamental constants from Big Bang to atomic clocks (theory and observations).*

Computational Spectroscopy

Organizers:

B.Champagne, U.Hohm,

G. Maroulis and C.Pouchan

Tuesday October 31, 2006 (Room 2)

Schedule	Speaker	Title of contribution
	Chair: S.Farantos	
9:00 – 9:30	W.Hug	Understanding Normal Modes of Molecules and Clusters
9:30-10:00	M.Fedorovsky	Exploring Vibrational Optical Activity with PyVib2
10:00-10:30	M.Reiher	Quantum chemical methods for the vibrational spectroscopy of large molecules
10.30 – 11.00	**COFFEE BREAK**	
	Chair: D.Begué	
11:00-11:30	V.Rodriguez	Hyper-Raman scattering in materials: towards high quality signals and spatial resolution
11:30 – 12:00	B.Champagne	*Ab Initio* Methods for Simulating and Interpreting hyper-Raman Spectra of Molecules
12:00 – 12:30	M.Hayashi	Sum Frequency Generation Chiral and Achiral Responses from Molecules in A Bulk Solution

Tuesday 31 October 2006 SESSION: COMPUTATIONAL METHODS CHAIR: D.S. VLACHOS (ROOM 2)		
16:00 – 16:30	*Josef Kapitán, Jiří Šebek and Petr Bouř*	**Different Effect of Solvent on Electronic and Vibrational Spectra**
16:30 – 17:00	*Chao Yang and Donald L. Koch*	**Effect of inertia on the mass/heat transfer from a neutrally buoyant sphere at finite Reynolds number in simple shear flow**
17:00 – 17:30	*Sunyoung Cho, Xuan Hung Ta, Chang No Yoon, Seung Kee Han*	**System Reduction Algorithm using Hierarchical Clustering for the Movement-related EEG Recognition**
Coffee Break		
18.00 – 18:30	*Chong Hyun Lee*	**Stochastic Modeling and Analysis of PLL Phase Noise on QAM based Communication System**
18:30 – 19:00	*Kuo Kan Liang , Jen Wei Yu and Sheng Hsien Lin*	**Theoretical Treatment of the Ultrafast Photo-Induced Electron Transfer in Dye-Sensitized Solar Cells**
19:00 – 19:30	*Chong Hyun Lee*	**Numerically Efficient Ranging Algorithm for UWB Communications**
19:30 – 20:00	*A. A. Lisin, D. V. Mogilenskikh, I. V. Pavlov*	**Nonlinear Color Interpretation of Physical Processes**
20:00 – 20:30	*Jinho Bae and Chong Hyun Lee*	**Circulant Matrix Factorization Applied for Designing FIR Lattice Filter Structures using Schur Algorithm**
20:30 – 21:00	*Marzieh Eskandari, Ali Mohades*	**The n-Round Voronoi Game**

Tuesday October 31, 2006 (Room 3)

Schedule	Speaker	Title of contribution
	Chair: J.Jellinek	
9.00 – 9.40	P.Jørgensen	Towards black-box linear scaling optimization in Hartree-Fock and Kohn-Sham theories
9.40-10.00	D.Xenides	Electric properties for HCCH, H_2CC, H_2CSi and H_2CGe
10.00-10.20	Yi Dong	Properties of Au_n Clusters
10.20-10.40	P.Karamanis	Structure and polarizability of small $(GaAs)_n$ clusters (n= 2, 3, 4, 5, 6, and 8)
10.40 – 11.00	**COFFEE BREAK**	
	Chair: S.Canuto	
11.00 – 11.40	M.Nakano	Theoretical Study on the Second Hyperpolarizabilities of Diphenalenyl Radical Systems
11.40 – 12.10	Y.Aoki	Elongation Method with Parallelization
12.10-12.30	D.Xenides	An ab initio and DFT study of the (hyper)polarizability of the C_4 and C_xSi_y (x+y=4) clusters
12.30-13.00	Li Zhi-Ru	Theoretical study on quantum mirage effect from a small quantum corral
13.00-13.20	M.P.Sigalas	*Ab initio* and Density Functional Theory Study of the Hydrogen - Bonded Pyridine - H_2S Complex
13.00-15.00	**LUNCH BREAK**	
	Chair: **M.Nakano**	
15.00-15.40	P.Mezey	Computational Quantum Chemistry Design of Nanospirals and Nanoneedles
15.40-16.10	T.Nanri	Implementation of GAMESS on Parallel Computers. TCP/IP versus MPI
16.10-16.40	M.Kosmas	On the activity and load capacity of dendritic block copolymers
16.40-17.00	**COFFEE BREAK**	
	Chair: **P.Mezey**	
17.00-17.25	N.I.Gidopoulos	Unconstrained Variational Determination of the Kohn-Sham Potential
17.25-17.45	M.Kabeláč	Trimers of Nucleic Acid Bases. Comparison of Empirical, DFT and High Level Correlated Ab initio Data with Experiment
17.45-18.10	H.Takahashi	A Novel Quantum Chemical Approach to the Free Energy Calculation for the One-electron Reduction of Coenzyme in Solution and Biological System
18.10-18.30	J.Zamastil	Algebraic methods in atomic calculations
18.30-18.50	P.Cysewski	Accurate gas phase acidities of carboxylic acids estimated by scaling of harmonic vibrational frequencies calculated on Hartree-Fock level.

Poster Session Tuesday 31/10/2006 19:00 – 21:00:

Li ZeSheng, S.Zalis, H.Berriche, Y.Kita, T.Udagawa, A.Hantzis, S.Jannsens

COMPUTATIONAL METHODS IN CHEMICAL ENGINEERING

Tuesday 31 October 2006 (Room 4)

Time	Authors	Title of Paper
11:30-12.00	G. D. Verros & A. K. Testempasi	An Alternative Proof of the Onsager Reciprocal Relations for Multi-component Diffusion
12.00-12.30	I.A. Bitsanis , A.N. Rissanou, M. Yannourakou, I.G. Economou, D. Vlassopoulos	Mesoscopic Simulations of T-Induced Solidification in Dense Suspensions of Ultrasoft Supramolecules
12.30-13.00	I. Prassa, P. Kontogeorgou, G. D. Verros, A. Koulouris and P. Samaras	Computer Aided Design and Optimization of an Incineration Plant for Slaughterhouse Wastes

Tuesday 31 October 2006

SESSION: COMPUTATIONAL METHODS
CHAIR:
J. MOC (ROOM 4)

16:00 – 16:30	*H. Torres-Silva*	**Ehhanced Absorption in Children Brain under Microwave Radiation**
16:30 – 17:00	*Piroz Zamankhan, Ali Halabia*	**Convective Motion in Shaken Sand**
17:00 – 17:30	*J. Moc*	**On the Hydrogenation of Gallium Trimer**
Coffee Break		
18.00 – 18:30	*S. Simić, D. Simić, P. Slankamenac*	**Integrating Case-based and Rule-based Decision Support in Headache Disorder**
18:30 – 19:00	*H. S. Sim, H. R. Gwon, Y. S. Cho, J. M. Kim, and S. H. Lee*	**Numerical Investigation on Ultrashort Pulse Laser Interactions with Thin Metal Film Structures Considering Quantum Effects**
19:00 – 19:30	*Piroz Zamankhan*	**Multiscale Modeling Approach in a Fiber Liquid Suspension**
19:30 – 20:00	*A. Shahsavand , A. Ahmadpour*	**Prediction of Energy and Pore Size Distributions Via Linear Regularization Theory**
20:00 – 20:30	*M. Ropotar, Z. Kravanja*	**Optimization of a Batch Reactor using NLP and MINLP**
20:30 – 21:00	*H. R. Gwon, H. S. Sim, S. Chae, S. H. Lee*	**Numerical Study on Optical Characteristics of Multi-Layer Thin Film Structures Considering Wave Interference Effects**

Tuesday 31 October 2006 SESSION: COMPUTER SCIENCE CHAIR: KENSUKE BABA (ROOM 5)		
09:00 – 09:30	*B. Boutsinas, Y. Nasikas*	**Document Clustering based on Association Rule Mining**
09:30 – 10:00	*J. Cervantes , C. Stephens*	**A Rank-Proportional Generic Genetic Algorithm**
10:00 – 10:30	*ByungRae Cha, JongGeun Jeong and HyunSook Chung*	**Digital License Design of S/W Source Code for IPR**
Coffee Break		
11.00 – 11:30	*Sang Il. Cho, Ern Yu. Lee, Tae Yong Kim, Hoon Jae Lee*	**A Threshold Clock-Control Summation Sequence Generator**
11:30 – 12:00	*Wonil Choi, JungHun Kang, XiaoYi Lu, Zhen Fu, Myong-Soon Park*	**Distributing Requests by Weighted Load Value in Cyber Foraging**
12:00 – 12:30	*Hanmei E, Yunqing Yu, Kensuke Baba and Kazuaki Murakami*	**Approximate String Matching Based on Bit Operations**
12:30 – 13:00	*JongGeun Jeong and ByungRae Cha*	**A Study on the Document Similarity Judgment using Similar Block Expansion**
13:00 – 13:30	*G. Hernandez and L. Salinas*	**NER Automata Dynamics on Random Graphs**
13:30 – 14:00	*Tianqiang Huang*	**Quick Density-based Approach to Identify Outliers**

Tuesday 31 October 2006 SESSION: COMPUTER SCIENCE CHAIR: HYEONG SEON YOO (ROOM 5)		
16:00 – 16:30	*Kugsang Jeong, Deokjai Choi*	**Providing Context Communication In Ubiquitous Computing Architecture**
16:30 – 17:00	*Jun Liang, Hyeong Seon Yoo*	**A Flexible ID-Based Group Key Agreement Protocol with Bilinear Pairings**
17:00 – 17:30	*Sang-Young Lee, Yun-Hyeon Lee*	**Workflow Engine for Mobile-Based Healthcare System**
Coffee Break		
18:00 – 18:30	*X. H. Liang, C. P. Wang*	**Layered Link List Based Marching Cubes Algorithm**
18:30 – 19:00	*Ulrich Norbisrath, Christof Mosler*	**Component-Based Development for eHome Systems**
19:00 – 19:30	*Sang-Young Lee, Suk-il Kim*	**Development of HIS System through the Integration of Legacy System**
19:30 – 20:00	*Jeoungpil Ryu, Jungseok Lee, and Kijun Han*	**A Probabilistic Approach on Topology Control in Wireless Sensor Networks**
20:00 – 20:30	*Zhao Qingling , Qian Ping , Su Xiaolu , Zhao Ming*	**Application of Ontology in Soil Knowledge Intelligent Retrieval System Based on Web**
20:30 – 21:00	*Zai-Sha Mao and Chao Yang*	**The Cell Model Approach to Solid Particle Assemblages: Further Justifications**
21:00 – 21:30	*B. Sadeghi Bigham, A. Mohades*	**The Dual of Polar Diagram and its Extraction**

Tuesday 31 October 2006	
SESSION: HIGHLIGHT LECTURES II **CHAIR: GEORGE MAROULIS (ROOM 1)**	
21:00 – 22:00	**Werner Kutzelnigg, University of Bochum, Germany**

Tuesday 31 October 2006

POSTER SESSION

21.00-23.00	1. L. Bayón, J. M. Grau, M. M. Ruiz, P. M. Suárez, The valve points of the thermal cost function: A Hydrothermal Problem with non-regular Lagrangian 2. E. F. Combarro, E. Montanes, I. Díaz, R. Contina, P. Alonso, J. Ranilla, NoW Architectures, Dimensionality Reduction and Self-Organizing Maps for Information Retrieval 3. Silvia Curteanu and Maria Cazacu, Neural networks based prediction and optimization applied to siloxane-siloxane copolymers synthesis 4. Y.-H. Liu, A Scatter Search Heuristic for an Econometric Model Estimation 5. F. Y. Yu and C. C Hung, An Empirical Analysis of Online Multiple-Choice Question-Generation Learning Activity for the Enhancement of Students' Cognitive Strategy Development While Learning Science 6. J. A. López, M. Barreda, J. Artés, High Performance Algorithms for the Management of the Poisson Series Developments in Celestial Mechanics 7. T. Rusu, M. Pinteala, S. C. Buraga, Computer Aid Design of Polydimethylsiloxanes Copolymer with Imposed Water Delivery Properties 8. J. Mateu, C. Comas, E. Porcu and J. A López, Probability Mapping in Cluster Spatial Processes. Computational and Analytical Solutions Through Copulas 9. G. P. Giatrakos, G. D. Naxakis, P. G. Mouchtaropoulos, T. D. Tsoutsos, Energy Planning and Cost Analysis of a Hydrogen - Saps System, Using Renewable Energy Sources, for Karpathos Island, Greece

Relativistic quantum theory: Computational perspectives and applications.

Crete, October 30 - November 1 2006

Wednesday November 1, 2006 (Room 1)

Schedule	Speaker	Title of contribution
	CHAIR : Martin Quack	
09.00 - 09.40	Christian Chardonnet (Paris, France)	*Towards a first observation of molecular parity violation by laser spectroscopy.*
09.40 - 10.10	Victor Flambaum (Sydney, Australia)	*Traditional Weak Interaction Physics in Atoms and Molecules.*
10.10 - 10.40	Robert Compton (Tennessee, USA)	*Experimental Searches for Minute Parity Violation Effects in Molecules.*
10.40 - 11.00	**COFFEE BREAK**	
	CHAIR : Robert Compton	
11.00 - 11.40	Martin Quack (Zürich, Switzerland)	*Theory and Molecular Spectroscopy of the Parity Violating Electroweak Interaction.*
11.40 - 12.10	Robert Berger (Frankfurt, Germany)	*Electroweak quantum chemistry: Do it Breit.*
12.10 - 12.40	Radovan Bast (Strasbourg, France)	*Parity non-conservation and NMR observables within the 4-component relativistic framework.*
12.40 - 13.10	Juergen Stohner (Zürich, Switzerland)	*Signatures from Electroweak Quantum Chemistry in Rovibrational Spectra of Polyatomic Molecules*
13.10 - 13.20	Peter Schwerdtfeger (Auckland, New Zealand)	*CONCLUDING REMARKS*
LUNCH		

Wednesday 1 November 2006

SESSION: COMPUTATIONAL AND MATHEMATICAL METHODS AND MODELLING
CHAIR:
DIONISSIOS T. HRISTOPULOS (ROOM 2)

09:00 – 09:30	*Aliki D. Muradova, Dionissios T. Hristopulos*	**Mathematical Modelling of Formation and Dissociation of Gas Hydrate in the Sea Floor Sediment**
09:30 – 10:00	*Nikos Pasadakis and Andreas A. Kardamakis*	**Classification of Gasoline Samples using Variable Reduction and Expectation-Maximization Methods**
10:00 – 10:30	*E. G. Vairaktaris, I. P. Vardoulakis*	**Modeling the Effect of Moisture Intrusion**
Coffee Break		
11.00 – 11:30	*Jari Niemi, Keijo Ruohonen and Ulla Ruotsalainen*	**Estimation of Physiologic Heterogeneity of Target Tissue in PET Studies Using Dynamic Compartment Models – Modification to Least-Squares Fit**
11:30 – 12:00	*Muhammad A. Mushref*	**Electromagnetic Scattering of *N* Plane Waves by a Circular Cylinder Coated with Metamaterials**
12:00 – 12:30	*Z. Nilforoushan, A. Mohades, A. Laleh, M. M. Rezaii*	**Voronoi Diagram in 3-D Hyperbolic space**
12:30 – 13:00	*Henryk Witek*	**Modeling nanostructures with the SCC-DFTB method**

Wednesday 1 November 2006

SESSION: COMPUTATIONAL AND MATHEMATICAL METHODS AND COMPUTER SCIENCE
CHAIR:
D.S. VLACHOS (ROOM 2)

16:00 – 16:30	*Wenbo Shi, Hyeong Seon Yoo*	**Improvement of a Secure Multi-Agent Marketplace**
16:30 – 17:00	*Jeongho Son, Jinsuk Pak, Hoseung Lee and Kijun Han*	**An Aggregation Point Determination Scheme for Wireless Sensor Networks with Multiple Sinks**
17:00 – 17:30	*Chang kun Song, Kyung seok Kim, Young hwan Lee and Dong won Jang*	**Performance Analysis of STBC/SFBC OFDM System on UWB Interferer**
Coffee Break		
18:00 – 18:30	*Jooseok Kim, Kyungseok Kim, Woogoo Park and Jinup Kim*	**Dynamic Spectrum Allocation Technique for Efficient Spectrum Sharing on Cognitive Radio environments**
18:30 – 19:00	*Li-Ran Shen, Qing-Bo Yin, Xue-Yao Li, Hui-Qiang Wang*	**Speech Stream Detection in Short-wave Channel Based on Two Dimension Image Analysis**
19:00 – 19:30	*A. Gómez-Corral M.E. Martos*	**Inter-departure times in a tandem G-queue with blocking**
19:30 – 20:00	*KyungSeok Kim and YoungJu Hyun*	**Blind Eigencanceler applying Hermitian Toeplitz method and the Higher-Order Cumulant method**
20:00 – 20:30	*J. Zamastil, M. Šimánek, F. Vinette*	**Algebraic methods in atomic calculations**
20:30 – 21:00	*Yeon-Mo Yang and Harry Perros*	**Centralized Control Message Transmission by using Multicast Burst Polling Scheme for QoS in EPONs**

Wednesday 1 November 2006

SESSION: COMPUTATIONAL AND MATHEMATICAL METHODS AND COMPUTER SCIENCE
CHAIR:
D.S. VLACHOS (ROOM 2)

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Wednesday 1 November 2006 SESSION: Neural Networks CHAIR: M.N. VRAHATIS (ROOM 3)		
09:00 – 09:30	*S. Adam, D. A. Karras, M. N. Vrahatis*	**A Study on Clustering Initial Weights Space of MLP Neural Networks in Terms of Fast Convergence and Generalization Capability**
09:30 – 10:00	*A. Ahmadpour , A. Shahsavand*	**Application of Neural Networks for Characterization of Porous Materials**
10:00 – 10:30	*M. G. Epitropakis, V. P. Plagianakos, M. N. Vrahatis*	**Integer Weight Higher-Order Neural Network Training Using Distributed Differential Evolution**
Coffee Break		
11.00 – 11:30	*V. L. Georgiou, Ph. D. Alevizos, M. N. Vrahatis*	**Incorporating Fuzzy Membership Functions into Evolutionary Probabilistic Neural Networks**
11:30 – 12:00	*A. Joghataie and M. Forrokh*	**Neural Networks in Analysis of Frames with Bouc-Wen Nonlinearity**
12:00 – 12:30	*A. Margaris and M. Roumeliotis*	**A General Purpose Parallel Neural Network Architecture**

Wednesday 1 November 2006 SESSION: COMPUTATIONAL METHODS AND MODELLING CHAIR: G.C. MELETIOU (ROOM 3)		
14:30 – 15:00	*E. K. Ikonomakis, D. K. Tasoulis, M. N. Vrahatis*	**Density Based Text Clustering**
15:00 – 15:30	*E. C. Laskari, G. C. Meletiou, M. N. Vrahatis*	**Designing S-boxes through Evolutionary Computation**
15:30 – 16:00	*Anwar-ul-Haque, Abdul Jabbar, Jawad Khawar, Sajid Raza Chaudhary*	**Role of Turbulence Modeling for Leading Edge Vortical Flow**
Coffee Break		
16.30 – 17:00	*N. G. Pavlidis, E. G. Pavlidis and M. N. Vrahatis*	**Genetically Programmed Trading Rules for the Foreign Exchange Market**
17:00 – 17:30	*V.P. Gkeleri and V. D. Tourassis*	**Disassemblability Metrics in the Design for Environment context**
17:30 – 18:00	*Alireza Haji, Babak Javadi and Kaveh Fallah Alipour*	**Application of Fuzzy Multi-Objective Linear Programming to No-Wait Flow Shop Scheduling**
18:00 – 18:30	*C. Martín-Sistac, G. Escudero and M. Graells*	**Efficient Management of Wastewater Treatment Networks**
18:30 – 19:00	*A. A. Niknafs , M. E. Shiri*	**Fuzzy-CBR Agent Design for Tourism Industry, A Multi Agent System Approach**
19:00 – 19:30	*M. E. Theocharis, C. D. Tzimopoulos, M. A. Sakellariou - Makrantonaki, S. I. Yannopoulos and I. K. Meletiou*	**Irrigation networks optimization using dynamic programming method and Labye's optimization method**
19:30 – 20:00	*Jang Mook Kang and Song Chul Moon*	**A Study on Privacy Enhancing Technologies of Radio Frequency Identification system in Ubiquitous Network Environment (Focus on Advanced and Emerging Security Engineering: Privacy Enhancing Technologies)**
20:00 – 20:30	*K.N. Genikomsakis and V.D. Tourassis*	**Integrating biased task assignment to balance an assembly line in a COMSOAL algorithm**
20:30 – 21:00	*Y. G. Petalas, C. G. Antonopoulos, T. C. Bountis and M. N. Vrahatis*	**Detecting Resonances using Evolutionary Algorithms**

Wednesday 1 November 2006

POSTER SESSION

19.00-21.00	1. P. Fariñas Alvariño, F. López Peña, Numerical and Experimental Study on a Submersible Catamaran Hydrodynamics 2. S. Bitamaa, R. Masmoudi, L. Messadia, H. Saadi, A. Ferhati, Protonation Sites of The two-substituted-4,6-di-(alkylamino)-1,3,5-triazines (s-triazines)-interaction with biological unit 3. Jang-Mi Baek, Dae-Hee Seo, A Study on Scalable Bluetooth Piconet based on Secure Inquiry Process for Ubiquitous Environment 4. Jang-Mi Baek, Dae-Hee Seo, A Study on RFID Authentication Protocol based on Secure Hash Function 5. Jianwei Li, Zhigang Lei , Biaohua Chen, Chengyue Li, CAMD for entrainer screening for separating 1-hexene and n-hexane 6. J. J. del Coz Díaz, P. J. García Nieto, J. A. Vilán Vilán and J. M. Matías Fernández, Non-linear analysis of a cold rolled forming thin-walled steel column by the finite element method

END OF THE CONFERENCE

We hope to see you next year

in ICCMSE 2007

2003 – 2007:
5 YEARS ICCMSE

ICCMSE 2006

INTERNATIONAL CONFERENCE OF COMPUTATIONAL METHODS IN SCIENCES AND ENGINEERING

CONFERENCE CONCERT

'Harmonic Oscillations between Classics and Pop'

MICHAEL TSCHUGGNALL

OCTOBER 28, 22.00

Programme

Europe

Mozart, Sonata C major

Tears of Happiness

Beautiful Thing

Life can be so hard

Beethoven, Sonata C Sharp Minor (Moonlight)

Song of Mine

Surprise Intermezzo

Bach, Fuga C minor

From the East

Schrödingers Equation