29 September 2009 Kirtman's symposium, SESSION: 1 CHAIR: Michael SPRINGBORG (ROOM 1)		
09:00 – 09:40	*Celso de Melo*	A Quantum Chemical Approach to the Molecular Conductance Problem
09:40 – 10:20	*Miquel Torrent-Sucarrat*	The Aplicability of the HSAB Principle
10:20 – 10:40	*Feng Long Gu*	Band Structure of Polymer Extracted from Oligomer Calculations by Elongation Method and Its Applications to Nanosystems
10:40 – 11:00	*Oleksandr Loboda*	Efficient algorithm for computing the orbital energies within elongation method
Coffee Break		
11:20 – 12:00	*Ajit Thakkar*	A hierarchy for additive models of polarizability
12:00 – 12:20	*Kikuo Harigaya*	Exciton Effects in Optical Absorption Spectra of Boron-Nitride Nanotubes
12:20 – 13:00	*Yuriko Aoki*	Generalization Elongation Method for Gigantic Systems of 1D, 2D, and 3D
13:00 – 13:20	*Violina Tevekeliyska*	Implementation of a vector potential method in *ab initio* Hartree-Fock code
Lunch Break		

29 September 2009 Kirtman's symposium, SESSION: 2 CHAIR: Feng Long GU (ROOM 1)		
15:00 – 15:20	*Roberto Dovesi*	Coupled perturbed HF/KS calculation of the polarizability of crystalline systems. The case of six members of the garnet family
15:20 – 15:40	*Michael Springborg*	On the dependence of bulk properties on surfaces
15:40 – 16:00	*Edith Botek*	Linear and nonlinear second-order susceptibilities of molecular crystals
16:00 – 16:20	*Bin PENG*	Homoleptic Mononuclear and Binuclear Ruthenium Carbonyls $Ru(CO)_n$ (n= 3-5) and $Ru_2(CO)_n$ (n = 9-6)
16:20 – 16:40	*Yi Dong*	Determining the size dependence of structural properties of clusters
16:40 – 17:00	*Aggelos Avramopoulos*	The effect of the vibrational contributions to the non-linear optical properties. Cases of small and medium size molecules
Coffee Break		
17:20 – 18:00	*Mauro Ferrero*	The Calculation of the Static Frst- and Second-Susceptibilities of Crystalline Urea. A Comparison of HF and DFT (LDA, GGA, hybrid) Results Obtained with the Periodic CP-HF/KS Scheme
18:00 – 18:20	*Heribert Reis*	Prediction of the linear and nonlinear electric susceptibilities of 3-methyl-4-nitropyridine-N-oxide (POM) and meta-nitroaniline (mNA) crystals with account of electronic and molecular vibrational contributions.
18:20 – 19:00	*Marek Wojcik*	Theoretical model for infrared spectra of hydrogen-bonded crystals
19:00 – 19:20	Jacek Korchowiec	Elongation cutoff technique at Kohn-Sham level of theory: an efficient sparse matrix algebra approach to linear scaling

29 September 2009 SESSION: Computational Quantum Chemistry The Symposium is dedicated to the memory of David M.Bishop (1936-2008) CHAIR: George Maroulis (ROOM 1)		
09:00 – 09:40	Trygve Helgaker	Accurate generalized adiabatic-connection curves
09:40 – 10:25	Markus Meuwly	Atomistic simulations for complex systems with chemical accuracy
10:25 – 11:05	Masayoshi Nakano	One- and Two-Photon Absorptions in Open-Shell Singlet Systems
Coffee Break		
11:30 – 12:10	Michael Dolg	**Efficient quantum chemical valence-only treatments of lanthanide and actinide systems**
12:10 – 12:50	K.L.C.Hunt	**Collision-Induced Dipoles and polarizabilities of Pairs of Hydrogen Molecules: *Ab Initio* Results and Spherical Tensor Analysis**
12:50 – 13:25	Ria Broer	**Quantum chemical study of the nature of the ground state in some transition metal perovskites**
Lunch Break		
CHAIR: Markus Mewly		
15:00 – 15:40	Jozef Noga	**Hartree-Fock Via Coupled Cluster Theory - A Way to Diagonalization Free Algorithm.**
15:40 – 16:20	Aristides Zdetsis	**The boron connection: Roots, grounds, horizons**
16:20 – 16:55	Pablo Villareal	**Quantum chemistry calculations in helium doped clusters**

Coffee Break		
CHAIR: Josef Noga		
17:30 – 18:10	**Weitao Yang**	**Development and application of ab initio QM/MM methods for simulation of chemical reactions in solution and in enzymes**
18:10 – 18:45	**Yuriko Aoki**	**Elongation Method for Linear Scaling**
18:45 – 19:20	**Xavier Assfeld**	**Electron addition on biomolecules: The disulfide case**
19:20 – 19:55	**Tadeusz Bancewicz**	**Can long-range collision-induced properties be modelled semi-classically?**
19:55 – 20:15	**I. Jendoubi**	**Theoretical study and formation prediction of the ultra-cold molecule RbLi**

29 September 2009 SESSION: Marie Curie Chair and European Science Foundation SUMMER SCHOOL 2009. ULTRAFAST DYNAMICS, STRUCTURE. TOWARDS BIOLOGICAL AND BIOMEDICAL APPLICATIONS CHAIR: Prof. Dr. Halina Abramczyk (ROOM 3)		
09:15 – 10:45	Günter Steinmeyer *Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopi, Berlin, Germany*	*Ultrafast pulse generation: basics and femtosecond oscillators*
11.00-11.15 Coffee Break		
11:30 – 13:00	Günter Steinmeyer *Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopi, Berlin, Germany*	*Ultrafast pulse generation: amplification and compression*
13:30 – 15:00 Lunch		
15:15 – 16:45	Rick Trebino *Georgia Tech School of Physics, Atlanta, Georgia, U.S.A*	*The Measurement of Ultrashort Laser Pulses*
17:00 – 17:15 Coffee Break		
17:15 – 18:15	Rick Trebino *Georgia Tech School of Physics, Atlanta, Georgia, U.S.A*	*Interferometric Techniques and Spatio-temporal Measurements*
18.30 – 20.00	Rick Trebino *Georgia Tech School of Physics, Atlanta, Georgia, U.S.A*	*FROG*

29 September 2009 Session: Ab initio and classical molecular dynamics simulations in molecular medicine and drug design CHAIR: Paolo Carloni (ROOM 4)		
11:00 – 11:30	Gianluca Lattanzi	Multiscale modeling and free energy calculations: from idealized biomolecules to the complexity of the cell environment.
11:30 –12:00	Cristian Micheletti	Dynamics-based alignment of enzymatic functional families: a novel scheme for comparing large-scale movements in proteins with same or different fold
12:00 –12:30	Feng Wang	Simulation of Electron Spectra for Nucleoside Antibiotics
12:30 – 13:00	Marco de Vivo	Enhanced Sampling Methods in Computational Drug Design
Lunch Break		
14:00-14:30	David Smith	Studying Enzymatic Mechanism with QM/MM Techniques: An Application to the Dehydration of Glycerol
14:30 – 15:00	Ursula Rothlisberger	Combining systems biology approaches with atomistic simulations: New routes for the sustainable production of chemical compounds
15:00 – 15:30	Giovanni Bussi	Folding proteins with explicit solvent molecular dynamics simulations
15:30 – 16:00	Olivia Pulci	TExcited state calculations in biological systems: Many-Body perturbation Theory meets QM/MM
16:00 – 16:30	Matteo Dal Peraro	Novel coarse grained potentials for multiscale molecular simulations of

		biological systems
17:00 – 17:15 Coffee Break		

29 September 2009 Session: Molecular Dynamics Simulations CHAIR: Xabier Lopez (ROOM 4)		
16:30 – 17:00	**Xabier.Lopez, Eider San Sebastian, Elyette Martin, Xabier Lopez, Annick Dejaegere, Roland H. Stote**	**Locating hotspots in the LFA1/ICAM1 AND LFA1/INHIBITOR interactions using molecular dynamics simulations**

29 September 2009 SESSION: Computing in Experimental High Energy Physics 1 CHAIR: Prof. Tulika Bose (ROOM 5)		
11:20 – 11:50	Roger Jones**	The ATLAS Computing Model
11:50 – 12:20	Paul Nilsson	Distributed Computing in ATLAS
12:20 – 12:50	Francisco Matorras	CMS Computing Model
Lunch Break		
15:00 – 15:30	Francesca Pastore	ATLAS Trigger : design and commissioning
15:30 – 16:00	Leonard Apanasevich	The CMS High-Level Trigger
16:00 – 16:30	Dirk Hufnagel	First few days in the life of CMS events
16:30 – 17:00	David Côté	Commissioning of the ATLAS reconstruction software with first data
17:00 – 17:15 Coffee Break		
17:15 – 17:45	Leonardo Sala	CRAB: Distributed analysis tool for CMS
17:45 – 18:15	Roger Jones**	Distributed Data Analysis in ATLAS

** => Speaker name to be confirmed by ATLAS experiment

29 September 2009 SESSION: Computational Mechanics for Solid Materials and Structures CHAIR: R. Kobayashi (ROOM 6)		
09:00 – 09:15	R. Kobayashi	Hybrid atomistic/coarse-grained-particle simulations of crack propagations
09:15 – 09:30	G. Milani	FE Limit Analysis Meso-mechanical Model For The Pushover Analysis Of 2D Masonry Frames
09:30 – 09:45	X.S. Zeng	Automated finite element modelling of 3D technical textiles
09:45 – 10:00	L.M. Zhang	The Vulnerability of Structures based on Energy Flow Networks
Coffee Break		

29 September 2009
20:15 ***Welcome Drink***

END OF THE 1ST DAY

30 September 2009 SESSION: Symposium on Computational Spectroscopy CHAIR: Peter Schwerdtfeger (ROOM 1)		
10:00 – 10:15	Introduction	Peter Schwerdtfeger
10:15 – 10:45	Detecting small effects in molecules: From nuclear hexadecapole coupling to parity violation and the change of fundamental constants in space-time	Peter Schwerdtfeger
Coffee Break		
11:30 – 12:00	Testing the time-invariance of fundamental constants using cold and not-so-cold molecules	Hendrick L. Bethlem, Paul Jansen, and Wim Ubachs
12:00 – 12:30	Theory and spectroscopy for ultracold KRb molecules	William Stwalley
12:30 – 13:00	Parity violating effects in diatomics and some group-theoretical considerations on chirality in polyatomic molecules	Robert Berger
13:30 – 15:00 Lunch Break		
15:00 – 15:30	An exact analytical model for He-like states of confined triatomics	Ulrich Müller-Herold
15:30 -16:00	Fully relativistic calculations of NMR and EPR parameters in the framework of the matrix Dirac-Kohn-Sham equation	Vladimir G. Malkin, Olga L. Malkina, Michal Repiský, and Stanislav Komorovský
16:00 -16:30	2- and 4-component relativistic studies of molecular electronic excited states	Trond Saue

30 September 2009 SESSION: Computing in Experimental High Energy Physics 2 CHAIR: Prof. Tulika Bose (ROOM 1)		
16:40 – 17:10	Tulika Bose	Review of Analysis Techniques in High Energy Physics
Coffee Break		
17:30 – 18:00	Jan Therhaag	TMVA: Toolkit for Multivariate Data Analysis
18:00 – 18:30	Roger Jones**	ATLAS Physics Analysis Tools
18:30 – 19:00	Roger Wolf	A tour of the CMS Physics Analysis Model
19:00 – 19:30	Matthias Edelhoff	CMS Alignment and Calibration Framework - Setup and First Experiences with Data
19:30 – 20:00	Monica Verducci	The Muon Conditions Data Management: Database Architecture and Software Infrastructure

** => Speaker name to be confirmed by ATLAS experiment

30 September 2009 Kirtman's symposium, SESSION: 3 CHAIR: Josep M. LUIS (ROOM 2)		
09:00 – 09:40	*Mark Hoffmann*	Generalized Van Vleck Perturbation Theory Study of Chlorine Monoxide
09:40 – 10:20	*Roberto Cammi*	On two recent developments of the Polarizable Continuum Model: squeezing molecules and correlating their electrons.
10:20 – 10:40	*Magdalena Pecul*	Environmental Effects on the Raman Optical Activity Spectra of Amino Acids: Theory and Experiment
10:40 – 11:00	*Elena Bogdan*	Experimental and Theoretical Investigations of Reference Molecules for Nonlinear Optics :The Example of Acetonitrile
Coffee Break		
11:20 – 12:00	*Kenneth Ruud*	Opening the Property Treasure Chest : a DFT Approach for Calculating Arbitrary Molecular Properties in the Relativistic and Nonrelativistic Domains
12:00 – 12:20	*Frédéric Castet*	Second-Order Nonlinear Optical Responses of Flexible Pyridine-Pyrimidine Foldamers
12:20 – 12:40	*Zhongzhi Yang*	Molecular Face Theory (MFT): The Topology Analysis of the (PAEM) and Local descriptors of reactivity mapping on the Molecular Face
12:40 – 13:00	*Robert Zalesny*	Critical assessment of density functional theory for computing vibrational (hyper)polarizabilities
Lunch Break		

30 September 2009 Kirtman's symposium, SESSION: 4 CHAIR: Benoît CHAMPAGNE (ROOM 2)		
15:00 – 15:40	*Ove Christiansen*	Vibrational Response Theory
15:40 – 16:00	*Josep M. Luis*	Nonlinear optical properties and large amplitude anharmonic vibrational motions
16:00 – 16:20	*Milena Spassova*	A DFT Study of the Second Hyperpolarizability of Linear ladder-type O-, N-, S-, and B-Fused Heterocyclic Oligomers
16:20 – 16:40	*Ryohei Kishi*	Long-Range-Corrected UDFT Study on Second Hyperpolarizabilities of Open-Shell Singlet Systems
16:40 – 17:00	*Kalju Kahn*	Anharmonic Vibrational Analysis Of Water At CCSD(T) Level: Comparison Of Traditional and Explicitly Correlated Methods
Coffee Break		
17:20 – 18:00	*Manthos Papadopoulos*	Novel Photonic Materials
18:00 – 18:20	*Benoît Champagne*	Bernie KIRTMAN in pictures

30 September 2009 SESSION: Computational Quantum Chemistry The Symposium is dedicated to the memory of David M.Bishop (1936-2008) CHAIR: Xavier Assfeld (ROOM 1)		
09:00 – 09:35	Sylvio Canuto	Electronic Spectroscopy and Reactivity of Molecules in Aqueous Environment.
09:35 – 10:10	Jacek Kobus	Overview of finite-difference Hartree-Fock method. Algorithm, implementation and application
10:10 – 10:45	Lasse Jensen	On the chemical enhancement in SERS
Coffee Break		
CHAIR: Sylvio Canuto		
11:40 – 12:25	Kizashi Yamaguchi	Theory of Chemical Bonds in Metalloenzymes -Manganese Oxides Clusters in the Oxygen Evolution Center-
12:25 – 13:00	Sourav Pal	Analytic energy derivatives for multi-root effective Hamiltonian theories: Polarizabilities and hyper-polarizabilities for radicals and excited states using coupled-cluster approach
13:00 – 13:35	Marianna Safronova	Atomic Calculations for Future Technology and Study of Fundamental Problems
Lunch Break		
CHAIR: Trygve Helgaker		
15:00 – 15:35	Trond Saue	Relativistic Hamiltonians for chemistry
15:35 – 16:10	Hajime Torii	Properties of Halogen Atoms for Representing Intermolecular

		Electrostatic Interactions Related to Halogen Bonding
16:10 – 16:50	Pratim Chattaraj	Conceptual Density Functional Theory Based Reactivity: Descriptors and Associated Electronic Structure Principles
Coffee Break		
CHAIR: Pablo Villareal		
17:30 – 18:05	Feng Wang	Simulating Ionization Spectra for Small Biomolecules in Inner and Valence Shells
18:05 – 18:40	Vincent Rodriguez	Vibrational Multipolar Analyses in isotropic media: Combining IR, Raman and Hyper-Raman spectroscopies
18:40 – 19:15	Bilge Demirkoz	Computing Challenges at the Large Hadron Collider at CERN
19:15 – 20:00	Bernard Kirtman	Calculation of the vibrational Contribution to Electronic Properties

30 September 2009 SESSION: 7th Symposium on Mathematical Chemistry *Dedicated to Professor Lionello Pogliani on the occasion of his 65th birthday* CHAIR: Sonja Nikolic, The Rugjer Boskovic Institute, Zagreb, Croatia (ROOM 4)		
09:00 – 09:05	Sonja Nikolic,	Introduction
09.05 - 09.25	Lionello Pogliani	A Metalanguage for Thermodynamics
09:25 – 09:45	Dusanka Janezic	New Protein-Protein Docking Methodology
09:45 – 10:05	Mario N. Berberan-Santos	A new approach to a century-old problem: Henri-Michaelis-Menten enzyme kinetics
10:25-10:50	Maria Rosaria Tiné	Adaptive modelling of structured molecular representations for toxicity prediction
10:50 - 11:10	Ramon Carbó-Dorca	Density Gradient Quantum Similarity
Coffee Break		
11:25 - 11:45	Sonja Nikolic	On additive version of the connectivity index
11:45 – 12:05	Henryk Chojnacki	Dipole Moment and Binding Energy in Positronic Molecules
12:05 – 12:25	Wilfried Gille	Analysis of randomly shaped puzzle-fragment-particles via their chord length distribution
12:25 – 12:45	Lech Schulz,	Chemistry as Mathematical System – Involutory Forms of Molecules and Their Genetic Codes
12:45 – 13:05	Gabriele Milani	Comparative numerical study on the optimal vulcanization of rubber compounds through traditional curing and microwaves
13:05 – 13:25	Paul G. Mezey	Discrete Skeletons of Continua in the Universal Molecule Model

30 September 2009 SESSION: New Frontiers in Modeling and Simulation of Composite and Metallic Field Machining CHAIR: M. EL-Mansori, H. A. Abdel-aal (ROOM 4)		
13:50 – 14:10	M. Calamaz, D. Coupard, F. Girot	Numerical simulation of Ti6Al4V titanium alloy dry machining
14:10 – 14:30	H.A. Abdel-Aal and M. El Mansori	Pressure-Induced Critical Influences on Workpiece-Tool Thermal Interaction in High Speed Dry Machining of Titanium
14:30 – 14:50	D. Iliescu, D. Gehin, I. Iordanoff, F. Girot	Discrete element method (DEM) modelling of the composite removal process
14:50 – 15:10	C. Espinosaa, J. Limidob, R. Chieragatti, C. Mabrua, M. Salaün, J. Lacomec	Use Of Orthogonal Cutting With SPH Method To Optimize The Cutting Design
15:10 – 15:30	L. Lasri, M. Nouri, M. EL Mansori	Numerical Simulation Of Progressive Failure And Chip Formation Process When Machining Fibre-Reinforced Polymer Composites

30 September 2009 SESSION: Computational aspects of the modelling of vibrational properties of gases, liquids and solids CHAIR: C. Pouchan (ROOM 4)		
15:30– 16:15	*J. M. Bowman*	Permutationally invariant Potential Energy Surfaces in high dimensionality and vibrational calculations using them.
16:15 – 17:00	*P. Tavan*	What the amide bands in the IR spectra of proteins and peptides can tell us: new computational methods and first applications.
Coffee Break		
17:15 – 17:45	*M. Hochlaf*	Benchmark calculations for the generation of multidimentional Potential Energy Surfaces of astrophysical and atmospheric relevant systems: theoretical treatment of N2H+ and related ions.
17:45 – 18:30	*D. Lauvergnat*	Quantum dynamics of floppy molecular systems with ELVibRot and Tnum
18:30 – 19:00	*M. Shiga*	Ab initio path integral simulations: nuclear quantum effect
19:00 – 19:30	*F. Gatti*	The importance of curvilinear coordinates in quantum dynamics and spectroscopy. Apllications to polyspherical approach.

19:30 – 20:00	***T. Carrington***	**Two new ideas for solving the vibrational Schrodinger equation: pruned product basis sets and neural network basis functions**
20:00 – 20:30	***E. Matito***	**Extrapolation of the potential energy surface using derivative information**
20:30 – 21:00	***O. Christiansen***	**Vibrational coupled cluster theory**
21:00 – 21:30	***W. Bian***	**Full-dimensional quantum dynamics study of resonance states of vinylidene using normal mode Hamiltonian**

30 September 2009 SESSION: Marie Curie Chair and European Science Foundation SUMMER SCHOOL 2009. ULTRAFAST DYNAMICS, STRUCTURE. TOWARDS BIOLOGICAL AND BIOMEDICAL APPLICATIONS CHAIR: Prof. Dr. Halina Abramczyk (ROOM 5)		
09:15 – 10:45	Shaul Mukamel *Chemistry Department University of California, Irvine, U.S.A*	*Principles of coherent multidimensional spectroscopy of molecules; quantum pathways of the wave function and density matrix*
11.00-11.15 Coffee Break		
11:30 – 13:00	Shaul Mukamel *Chemistry Department University of California, Irvine, U.S.A*	*Probing coherent and incoherent energy transfer in photosynthetic complexes by multidimensional optical techniques*
13:30 – 15:00 Lunch		
15:15 – 16:45	R. J. Dwayne Miller Department of Physics University of Toronto, Ontario, Canada	*Making the Molecular Movie: The Quest for the Structure-Function Correlation of Biology*
17:00 – 17:15 Coffee Break		
17:30 – 19:00	R. J. Dwayne Miller Department of Physics University of Toronto, Ontario, Canada	*Do We Live in a Quantum World? A New Twist. Quantum State Dynamics Relevant to Biological Systems*

30 September 2009 SESSION 1: Open-Shell Molecules, Graphenes and Conjugated Molecules I CHAIR: M. Nakano (ROOM6)		
10:00 – 10:20	*Takashi Kubo*	Singlet Open-Shell Character of Conjugated Kekulé Molecules
10:20 – 10:40	*Yasukazu Hirao*	Synthesis and Electronic Structure of Bisanthene: A Small Molecular-Sized Graphene with Zigzag Edges
10:40 – 11:00	*Yasutaka Kitagawa*	Vibrational frequency without Spin Contamination Error - Approximately Spin Projected Force Constant -
Coffee Break		
SESSION 1: Open-Shell Molecules, Graphenes and Conjugated Molecules I CHAIR: K. Harigaya		
11:20 – 11:40	*Katsunori Wakabayashi*	Electronic Transport of Graphene Nanoribbons: Effect of Edges and Geometry
11:40 – 12:00	*Pedro Henrique de Oliveira Neto*	Electron Correlation and Chain Relaxing Effects on the Graphene Energy Spectrum
12:00 – 12:20	*Geraldo Magela e Silva*	Polaron Dynamics in Graphene Nanoribbons
12:20 – 12:40	*Wiliam Ferreira da Cunha*	Charge Carrier Untrapping by Temperature Effects in Conjugated Polymers
13:00 – 13:20	*Ken-ichi Sugiura*	Synthesis and Theoretical Studies on π-Conjugated Cyclic Porphyrin Oligomers

30 September 2009 SESSION 2: Open-Shell and Conjugated Molecules: Electromagnetic Properties and Electron/Spin Transport CHAIR: H. Takahashi (ROOM6)		
15:00 – 15:20	*Masahiko Hada*	Magnetic Shielding in Carbon Nanotube
15:20 – 15:40	*Daisuke Yamaki*	Quantum-chemical analysis of paramagnetic ^{13}C NMR shifts of iron-bound cyanide ions in heme-protein environments
15:40 – 16:00	*Edith Botek*	Theoretical investigation of the ESR spectra of nitroxyl radicals
SESSION 2: Open-Shell and Conjugated Molecules: Electromagnetic Properties and Electron/Spin Transport CHAIR: K. Harigaya		
16:00 – 16:20	*Haibin Su*	Multi-Paradigm Simulations at the Nanoscale: Methodology and Applications to Functional Carbon Materials
16:20 – 16:40	*Ricardo Gargano*	Spin Transport in π-Conjugated Poly(*p*-Phenylene Vinylene) Polymers
16:40 – 17:00	*Hitoshi Fukui*	Second Hyperpolarizabilities of Singlet Diradical Compounds and Their Radical Ions
17:00 – 17:20	*Ryohei Kishi*	Broken-Symmetry MO-CI Quantum Master Equation Approach to Exciton Dynamics in Open-Shell Singlet Systems

30 September 2009 SESSION 3: Open-Shell and Conjugated Molecules: Optical Properties and others CHAIR: T. Kubo (ROOM6)		
18:00 – 18:40	*Masahiro Ehara*	Optical properties and electronic structures of conjugated molecules: SAC-CI study
18:40 – 19:00	*Takao Tsuneda*	A Multiconfigurational Density Functional Theory
19:00 – 19:20	*Masayoshi Nakano*	Spin Polarization and Third-Order Nonlinear Optical Properties of Open-Shell Singlet Graphene Nanoflakes
19:20 – 19:40	*Hideaki Takahashi*	Electron Donor Solvent Effects on the (Hyper)Polarizabilities of a Solute Presenting Singlet Diradical Character
19:40 – 20:00	*Yasuteru Shigeta*	I-V characteristics of several modified DNA bases

30 September 2009 SESSION: Properties of Metal 1,2-dithiolene and related compounds CHAIR: Aggelos Avramopoulos (ROOM 7)		
10:15-10:40	Reizo Kato	Conducting and magnetic properties of metal 1,2-dithiolenes
10:40:11:05	Marat Khusniyarov	Electronic structure of highly covalent coordination compounds of iron with redox-active a-diimine ligands
Coffee Break		
11:20 – 11:45	Wrochem von Floria	Dithiocarbamate-metal complexes and their impact on charge transport: a prospect for future molecular electronic devices
11:45 – 12:10	Masayoshi Nakano	Third-order nonlinear optical properties of square planar metal complexes involving o-semiquinonato type ligands
12:10-12:35	Pina Romaniello	Non linear optical properties of metal-dithiolenes
12:35 – 13:00	Francesco Lelj	Linear and nonlinear optical properties of Ni[Me6pzS$2]MX (M=Ni, Pd, Pt; X=Me2timdt, mnt
Lunch Break		

30 September 2009 SESSION: Theory and applications of organometallic compounds CHAIR: Heribert Reis (ROOM 7)		
15:30-15:55	Marcel Swart	Accurate description of spin states and its implications for catalysis
15:55 – 16:20	Ferran Feixas	Theoretical Evaluation of Electron Delocalization in Organometallic Compounds: From Agostic Bond to Aromaticity
16:20-16:45	Juan F. Van der Maelen Uría	A comparative topological study of different metal-metal and metal-ligand interactions in polynuclear organometallic clusters
Coffee Break		
18:15-18:40	Xavier Solans Monfort	Mechanistic insights in silica supported olefin metathesis catalysis: The role of the metal and ligands in catalyst activity and deactivation
18:40-19:05	Vidar R. Jensen	Systematic use of electronic structure theory in catalyst design
19:05-19:30	Ruben Mario	Surface-confined Coordination Chemistry

END OF THE 2nd DAY

1 October 2009 Kirtman's symposium, SESSION: 5 CHAIR: Celso de MELO, (ROOM 1)		
09:00 – 09:40	*Miquel Sola*	On the Reliability of the Maximum Hardness and Minimum Polarizability Principles in Nontotally Symmetric Vibrations
09:40 – 10:20	*Weitao Yang*	Insight and Progress in Density Functional Theory
10:20 – 10:40	*Michael Springborg, Josep M. Luis, Feng Long Gu, and Benoît Champagne*	Closing of Bernie Kirtman's symposium
Coffee Break		

1 October 2009 Distinguished Lecture CHAIR: Prof. G. Maroulis (ROOM 1)		
09:00 – 10:00	*Paul G. Mezey*	Molecular Modeling and the Violation of Linear Scaling Principles

1 October 2009 Distinguished Lecture CHAIR: Prof. G. Maroulis (ROOM 1)		
10:00 – 11:00	*Ernest R. Davidson*	Variational Definitions of Orbital Energies

1 October 2009 Distinguished Lecture CHAIR: Prof. G. Maroulis (ROOM 1)		
11:00 – 12:00	*Werner Kutzelnigg*	Rate of Convergence of Basis Expansions in Quantum Chemistry

1 October 2009 Distinguished Lecture CHAIR: Prof. G. Maroulis (ROOM 1)		
12:00 – 13:00	*George C. Schatz*	Nanoparticles, DNA and Theory

1 October 2009
13:15 **Photo of the Conference**

1 October 2009
13:30 **Excursion**

1 October 2009
20:15 **Central Dinner**

END OF THE 3rd DAY

2 October 2009 SESSION: Symposium on Computational Spectroscopy CHAIR: P. R. Bunker (ROOM 1)		
9:00 – 9:15	P. R. Bunker	Introduction
9:15 – 9:45	P. R. Bunker, W. P. Kraemer, Tsuneo Hirano and Per Jensen	Renner effect in triatomic molecules
9:45 – 10:15	Andreas Hauser, Carlo Callegari and Wolfgang E. Ernst	The Jahn-Teller effect and spin-orbit coupling in heavy alkali trimers: spectroscopic experiments and ab initio calculations
10:15 – 10:45	Xiao-Gang Wang and Tucker Carrington Jr.	Rovibrational spectra of molecules in small helium clusters
COFFEE BREAK		
11:30 – 12:00	Sergei N. Yurchenko, Walter Thiel and Per Jensen	Rotation-vibration energy level cluster formation in three- and four-atomic molecules
12:00 – 12:30	Ad van der Avoird, Rob van Harrevelt, Claude Leforestier, Rafal Podeszwa, Krzysztof Szalewicz, P. R. Bunker, Gert von Helden, Melanie Schnell and Gerard Meijer	Rovibrational and tunneling states of the benzene dimer: An ab initio study
12:30 – 13:00	Undine Erlekam, Gerard Meijer and Gert von Helden	Infrared spectroscopic and ab initio studies of the benzene dimer
LUNCH BREAK		

2 October 2009 SESSION: Symposium on Computational Spectroscopy CHAIR: P. R. Bunker (ROOM 1)		
15:00 – 15:30	Peter Botschwina and Rainer Oswalda	High-level ab initio calculations for (potential) interstellar anions: structures, spectroscopic properties and energetics
15:30-16:00	Stuart Carter, Joel M. Bowman, and Amit R. Sharma	The `MULTIMODE' approach to rovibrational spectroscopy
16:00-16:30	Jinjun Liu, Daniel Sprecher, Frédéric Merkt, Edcel J. Salumbides and Wim Ubachs	Measurement of the ionization and dissociation energies of H_2 and He_2
16:30-17:00	Feng Wang	Simulating ionization spectra of small biomolecules in inner and valence shells

Thursday 2 October 2009 Kirtman's symposium, SESSION: 5 CHAIR: Celso de MELO (ROOM 2)		
09:00 – 09:40	Miquel Sola	On the Reliability of the Maximum Hardness and Minimum Polarizability Principles in Nontotally Symmetric Vibrations
09:40 – 10:00	Michael Springborg, Josep M. Luis, Feng Long Gu, and Benoît Champagne	Closing of Bernie Kirtman's symposium
Coffee Break		

2 October 2009 SESSION: Computational and Mathematical Methods I CHAIR: Edward Karavakis (ROOM 2)		
16:30 – 17:00	Edward Karavakis and Akram Khan	A Multi-Threaded and Distributed Framework for Pedestrian Simulation Analysis

2 October 2009 SESSION: Computing in Experimental HEP 3 CHAIR: Prof. Tulika Bose (ROOM 2)		
11:20 – 11:50	Daniele Trocino	The CMS Muon Reconstruction Software
11:50 – 12:20	Thomas Punz	The CMS ECAL data handling
12:20 – 12:50	Karolos Potamianos	Data quality monitoring of the CMS Tracker
Lunch Break		
15:00 – 15:30	Edward Karavakis	CMS Dashboard for Monitoring of the user analysis activities
15:30 – 16:00	Salvatore Di Guida	Web application for detailed real-time database transaction monitoring for CMS condition data
16:00 – 16:30	Antonio Pierro	A machine learning approach to error detection in a database transaction system.

02 Octoberber 2009 SESSION: Computational aspects of the modelling of vibrational properties of gases, liquids and solids CHAIR: P. Carbonniere (ROOM 3)		
09:15 – 10:00	*K. Yagi*	*Vibrational quasi-degenerate paerturbation theory: Applications to nucleic acid base pairs*
10:00 – 10:30	*H. Torii*	Time-domain calculations of the the 1D and 2D spectra of resonantly-coupled vibrations in liquids and proteins.
10:30 – 11:00	*A. Ghysels*	Normal mode analysis of macromolecular systems with the mobile block Hessian method
Coffee Break		
11:15 – 11:45	*D. Janezic*	Hamiltonian splitting methods for macromolecular simulations
11:45 – 12:15	*B. Champagne*	Simulating and interpreting vibrational spectra of molecules
12:15 – 12:45	*D. Schofield*	Vibrational spectroscopy as a probe of relative energetics in flexible biomolecules.
12:45 – 13:15	*H. G. Bohr*	Computation of vibrational spectra of small peptides.

2 Octoberber 2009 SESSION: Computational aspects of the modelling of vibrational properties of gases, liquids and solids CHAIR: R. Dovesi (ROOM 3)		
15:15 – 15:45	*A. Pasquarello*	Medium range structure of disordered oxides through the first principles. Investigation of vibrational spectroscopies.
15:30 – 16:00	*E. Dolgusheva*	Vibrational spectra and anharmonic effects in crystals studied by molecular dynamics simulation
16:00 – 16:30	*A. D'Al Corso*	Recent devlopments in density functional perturbation theory
16:30 – 17:00	*X. Gonze*	Implementation of Density functional perturbation theory within ABINIT: Projector-Augmented Waves and Spin-Orbit.
Coffee Break		
17:15 – 17:45	*F. Gaspari*	Computational experiment in non-crystalline materials from first-principles: a case study of vibrations in hydrogenated amorphous silicon.
17:45 – 18:30	*R. Dovesi*	Quantum mechanical simulation of the vibrational properties of cristalline solids and interpretation of modes. The case of garnets and related minerals.
18:30 – 19:00	*C. Pouchan or P. Carbonniere*	Vibrational treatment from a variation-perturbation scheme: the VCI-P method

2 October 2009 SESSION: Marie Curie Chair and European Science Foundation SUMMER SCHOOL 2009. ULTRAFAST DYNAMICS, STRUCTURE. TOWARDS BIOLOGICAL AND BIOMEDICAL APPLICATIONS CHAIR: Prof. Dr. Halina Abramczyk (ROOM 4)		
10:00 – 10:45	**Halina Abramczyk Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopi, Berlin, Germany**	***Linear and Nonlinear Optical Methods for the Determination of Structure and Dynamics of Human Cell. Raman markers of breast cancer***
11.00-11.15 Coffee Break		
11:30 – 12:30	**Halina Abramczyk Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopi, Berlin, Germany**	*Advances in ultrafast spectroscopies refine our understanding of quantum coherences, role of weak interactions and structural dynamics of biological systems: bacteriorhodopsin, lipid membranes and breast cancer* ***tissue***
13:30 – 15:00 Lunch		
15:15 – 16:45	**Stavros C. Farantos Department of Chemistry, University of Crete, Iraklion Crete, Greece**	**Energy Localisation in Molecules, Bifurcation Phenomena, and their Spectroscopic Signatures**
17:00 – 17:15 Coffee Break		
17.30 – 18.15	**Albrecht Lindinger Institut für Experimentalphysik, Freie Universität Berlin, Berlin, Germany**	***Simultaneous phase, amplitude, and polarization control of femtosecond laser pulses***

2 October 2009 SESSION 4: Open-Shell Molecules, Graphenes and Conjugated Molecules II CHAIR: K. Wakabayashi (ROOM 5)		
09:00 – 09:40	*Mikito Koshino*	Giant Diamagnetism in Graphenes
09:40 – 10:00	*Kikuo Harigaya*	Edge States and Possible Magnetic States in Open-Shell Conjugated Systems
10:00 – 10:20	*Hirofumi Sato*	Coronene-transition metal complex: view from quantum chemistry and statistical mechanics
Coffee Break		
SESSION 4: Open-Shell Molecules, Graphenes and Conjugated Molecules II CHAIR: K. Harigaya		
11:20 – 11:40	*Benoît Champagne*	Theoretical Aspects on the Evaluation and Interpretation of the Third-Order Nonlinear Optical Properties of Diradical Compounds
11:40 – 12:00	*Shyusuke Yamanaka*	Locality and Nonlocality of Electronic Structures of Molecular Systems: Toward QM/MM and QM/QM approaches
12:00 – 12:20	*Ken-Ichiro Imura*	Z_2 classification of localization properties in graphene
12:20 – 12:40	*Ken-Ichiro Imura*	Spin-Orbit Effects in a Graphene Bipolar p-n Junction

2 October 2009 SESSION: Computational and Mathematical Methods II CHAIR: M. Martínez-Gómez (ROOM 6)		
14:30 – 14:45	Marí-Benlloch, M.; Martínez-Gómez, M.; Maroto, C; Suárez, J; Crespo, F.	Characterization of Forest Fires in Mediterranean Area
14:45 – 15:00	Georgy I. Burde, Alexander Zhalij, Ildar Sh. Nasibullayev	A new technique in the stability analysis of nonparallel flows

2 October 2009 SESSION: In the cage! Theoretical and computational studies of endohedral complexes and nanostructures CHAIR: Bartłomiej Skwara (ROOM 6)		
15:00-15:25	*Robert Góra*	On The Influence Of Intermolecular Interactions On The Static Electric Properties Of The Model Endohedral Complexes of Rare Gas Atoms.
15:25-15:50	*Oleksandr Loboda*	To be announced
15:50-16:15	*Bartłomiej Skwara*	Linear and Nonlinear Electric Properties of selected endohedral fullerenes.

2 October 2009 SESSION: Natural gas hydrates, a future climate bomb or a valuable source of energy? Opportunities and challenges for the computational physics community CHAIR: Bjørn Kvamme (ROOM 7)		
09:00 – 09:15	**Tatiana Kuznetsova, Bjørn Kvamme, Kathryn Morrissey**	**An alternatives for carbon dioxide emission mitigation: *in situ* methane carbon conversion**
09:15 – 09:30	**Norbert Lümmen and Bjørn Kvamme**	Molecular dynamics simulations of nucleation and growth of mixed $FeCl_2$/NaCl nanoparticles from supercritical water
09:30 – 09:45	**Tatiana Kuznetsova, Bjørn Kvamme, Archana Parmar**	Molecular dynamics simulations of methane hydrate pre-nucleation phenomena and the effect of PVCap kinetic inhibitor
09:45 – 10:00	**Bjørn Kvamme, Khuram Baig, Muhammad Quasim**	**Phase Field Theory modelling of methane fluxes from exposed natural gas hydrate reservoirs**
10:00 – 10:15	**Bjørnar Jensen, Bjørn Kvamme, Tatyana Kuznetsova, Åge Oterhals**	Modelling trapping mechanism for PCB adsorption on activated carbon
10:15 – 10:30	**Bjørn Kvamme, Tatyana Kuznetsova, Martin Haynes**	**Molecular dynamics studies of water deposition on hematite surfaces**
11:00 Coffee Break		

END OF THE 4th DAY

3 October 2009
SESSION: Computational Quantum Chemistry
The Symposium is dedicated to the memory of David M.Bishop (1936-2008)
CHAIR: Vincent Rodriguez
(ROOM 1)

09:00 – 09:25	Aristides D. Zdetsis	Silicon "Fullerenes"? Results and Expectations
09:25 – 09:50	A.Elias	The characterization of point defect distributions on linear collision sequences (LCS) in bcc tantalum.
09:50 – 10:15	Bao-Xing Li	Oxidation reactions of H_2O and N_2O with Si clusters: A first principles study
10:15 – 10:40	K.Harigaya	Exciton Effects in Boron-Nitride (BN) Nanotubes
10:40 – 11.05	Majid Hashemianzadeh	Adsorption and reactivity of H, H_2, CO, Adenine on Li-BNNT with and without Stone-Wales (SW) defect
Coffee Break		
CHAIR: Kikuo Harigaya		
11:30 – 11:55	Panaghiotis Karamanis	Is There Any Connection Between The (Hyper) Polarizabilities Of The Ground State Structures Of Clusters And Those Of Their Low Lying Isomers? A case study Of Aluminum Doped Silicon Clusters.
11:55 – 12:20	M. Korek	Ab initio Calculation of Molecular States of Compounds of the Lanthanum and Yttrium Molecules.
12:20 – 12:45	T.Minami	Oscillatory and Rotatory Exciton Recurrence Motions in Double-Ring Molecular Aggregates Controlled by Two-Mode Circular-Polarized Laser Field
Lunch Break		

CHAIR: Yuriko Aoki		
15:00 – 15:25	**Jean-Philip Piquemal**	**Understanding many-body interactions in biomolecules: from peptides to metalloenzymes**
15:25 – 15:50	**M.Swart**	**A New DFT Functional Based On Spin-states And SN2 Barriers**
15:50 – 16:15	**N.Vaval**	**Excited state molecular properties using constrained variational Fock space multireference coupled cluster**
16:15 – 16:40	**I.Paidarova**	**A comparison of density unctional theory and coupled cluster methods for the calculation of electric dipole polarizability gradients of methane**
Coffee Break		
CHAIR: Trond Saue		
17:30 – 17:55	**Philippe Carbonniere**	**Global Search Algorithm of Minima Exploration to Find Low Lying Isomers of clusters in Which Spheroidal Generation and Raking Optimization Appear As an Original Process.**
17:55 – 18:20	**Aristides D. Zdetsis and Emmanuel N. Koukaras**	**Theoretical study of $Si_{20}Li_{20}$ cage cluster**

3 October 2009 SESSION: Marie Curie Chair and European Science Foundation SUMMER SCHOOL 2009. ULTRAFAST DYNAMICS, STRUCTURE. TOWARDS BIOLOGICAL AND BIOMEDICAL APPLICATIONS CHAIR: Prof.Dr.Halina Abramczyk (ROOM 2)		
10:00 – 10:45	Thomas Elsaesser Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopi, Berlin, Germany	*Ultrafast structural dynamics of condensed matter studied by femtosecond x-ray methods*
15:30 – 17:00	Poster session	

3 October 2009 SESSION 23: 6th Symposium on Industrial and Environmental Case Studies CHAIR: Fragiskos Batzias (ROOM 3)		
	Presenter	***Title***
15:00 – 15:15	**Y.A. Pollalis**	***Tracing the transition path between optimal strategies combinations within a competitive market of innovative industrial products***
15:15 – 15:30	**M. F. Teodoro**	***Industrial production index forecast: Methods comparison***
15:30 – 15:45	**D. Sidiras**	***Simulation of acid hydrolysis of lignocellulosic residues to fermentable sugars for bioethanol production***
15:45 – 16:00	**D. Politi**	***Chromium (VI) purification using pine sawdust in batch systems***
16:00 – 16:15	**L. Beneš**	***Numerical Simulation Of The Neutrally Stratified ABL Flow Over Complex Geometry***
16:15 – 16:30	**K. Ifanti**	***Introducing economic parameters in industrial flotation dimensionless models used for intra-factory technology transfer***
16:30 – 16:45	**C. Siontorou**	***On the optimal design of molecular sensing interfaces with lipid bilayer assemblies – A knowledge based approach***
16:45 – 17:00	**O. Kopsidas**	***Evaluating environmental impact caused by industrial activities – Implementation of the WTP-WTA aproach***
Coffee Break		

Posters

- ***A Generalized Model For Simulating Adsorption On Porous Media And Checking For Reversibility By Desorption***
  Athanasia Bountri, Fragiskos Batzias, Dimitris Sidiras
- ***Searching For Correspondence Between Mechanismic/ Deductive And Empirical/Inductive Models At Industrial Level By Means Of Dimensional Analysis***
  Athanasia Bountri, Fragiskos Batzias, Dimitris Sidiras
- ***Endogenous Estimation Of Safety Coefficient For Optimal Design Of Biochemical Reactors At Industrial Level***
  Christina G. Siontorou and Aggeliki Karidi
- ***Computer Aided Design of Medicinal Products Based On Interactive Chemical/Herbal Ingredients – An R&D Approach***
  Christina G. Siontorou
- ***Analytic Estimation of Recycled Products Added Value As A Means For Effective Environmental Management***
  Dimitris F. Batzias
- ***Transforming Incomplete Fault Tree To Ishikawa Diagram As An Alternative Method For Technology Transfer***
  Dimitris F. Batzias
- ***Technology Transfer By Means Of Fault Tree Synthesis***
  Dimitris F. Batzias
- ***Technology Transfer Through A Network Of Standard Methods And Recommended Practices – The Case Of Petrochemicals***
  Dimitris F. Batzias and Sotirios Karvounis
- ***Industrial Wastewater Treatment In Fixed-Bed Systems***
  Dimitris Tsatiris and Dimitris Sidiras
- ***Parameter Identification of Process Simulation Models As A Means For Knowledge Acquisition And Technology Transfer***
  Dimitris F. Batzias and Konstantina Ifanti
- ***Introducing A Conditional 'Willingness To Pay' Index As A Quantifier For Environmental Impact Assessment***
  Odisseas Kopsidas and Fragiskos Batzias
- ***Determination Of Optimal Environmental Policy For Reclamation Of Land Unearthed In Lignite Mines – Strategy And Tactics***
  Dimitris F. Batzias and Yannis A. Pollalis
- ***The Analytic Solution of the Firm's Cost-Minimization Problem with Box Constraints and the Cobb-Douglas model***
  L. Bayón, J.M. Grau, M.M. Ruiz and P.M. Suárez,
- *Non-linear analysis and calculation of the performance of a shelving protection system by FEM*
  P.J. García Nieto, J.J. del Coz Díaz, J.A. Vilán Vilán and J.L. Suárez Sierra
- *Non-linear thermal analysis of the efficiency of light concrete big-holed bricks by FEM*
  J.J. del Coz Díaz, P.J. García Nieto, A. Lozano Martínez-Luengas and J. Domínguez Hernández

3 October 2009 SESSION: Recent Developments in Numerical Schemes for Hilbert Space Related Issues in Science and Engineering CHAIR: Metin Demiralp (ROOM 4)		
09:00 – 09:45	Metin Demiralp	Various Parallel and Diversive Aspects of the Mathematical Fluctuations Theory with the Standing Related Issues
09:45 – 10:00	Ercan Gurvit, N. Abdulbaki Baykara and Metin Demiralp	Fluctuation Studies in the Finite Interval Matrix Representations of Operator Products and Their Decompositions
10:00 – 10:15	N. Abdulbaki Baykara, Ercan Gurvit and Metin Demiralp	Fluctuation Studies in the Infinite Interval Matrix Representations of Operator Products and Their Decompositions
10:15 – 10:30	Cosar Gozuk?rm?z? and Metin Demiralp	Self-consistent Fluctuation Expansion And Its Application To Numerical Integration
10:30 – 10:45	Muzaffer Ayvaz and Metin Demiralp,	Optimal Control Equations for the One Dimensional Quantum Harmonic Oscillator Under the Influence of External Dipole Effects
10:45 – 11:00	Sergei Manzhos and Tucker Carrington	Representing potential energy surfaces with neural networks and high dimensional model representations
Coffee Break		
11:15 – 11:30	M. Tuba Gulpinar, Caner Gulpinar and Metin Demiralp	Exponentially Supported Polynomial Basis Set Using Fluctuation Free Integration in the Taylor Expansion Remainder Term Evaluation

11:30 – 11:45	Dana ?Cern? and V?clav Fin?ek	AdaptiveWavelet Methods – Matrix-Vector Multiplication
11:45 – 12:0	Caner Gulpinar, M. Tuba Gulpinar and Metin Demiralp	Taylor Series Expansion with the Fluctuation Freely Approximated Remainder over Gauss Wave Type Basis Functions
12:00 – 12:15	Suha Tuna, N. Abdulbaki Baykara and Metin Demiralp	Taylor Series Based Integration With The Fluctuation Freely Approximated Remainder Over Gauss Wave Type Basis Functions
12:15 – 12:30	Burcu Tunga and Metin Demiralp	Support Function Influences on the Univariance of the Enhanced Multivariance Product Representation
12:30 – 12:45	Sevda Uskuplu and Metin Demiralp	Basic Components in Fluctuation Free Integration of Highly Oscillatory Functions
12:45 – 13:00	Evrim Korkmaz and Metin Demiralp	Data Completion Via Combined and Optimized Small Scale High Dimensional Model Representation
13:00 – 13:15	M. Alper Tunga and Metin Demiralp	Fluctuation Free Matrix Representation Based Random Data Partitioning Through HDMR

3 October 2009 SESSION: Recent Developments in Numerical Schemes for Hilbert Space Related Issues in Science and Engineering CHAIR: Metin Demiralp (ROOM 4)		
14:15 – 14:30	Metin Demiralp and Emre Demiralp	Dimensionality Reduction And Approximation Via Space Extension And Multilinear Array Decomposition
14:30 – 14:45	L. Dihoru, C. A. Taylor, S. Battacharya, D. Muir Wood, A. Simmonelli, F. Moccia, G. Mylonakis	A neural network model for the maximum bending response of a pile under seismic loading
14:45 – 15:00	M. López, J. Taboada, J. Martínez, J.M. Matías , and J.A. Vilán	Slate Characterization Using 3D Laser Scanning
15:00 – 15:15	I. Marín, E. Arias, M. M. Artigao and J.J. Miralles	High Performance Implementations for Computing the Maximal Lyapunov Exponent on Distributed Memory Architectures
15:15 – 15:30	J.A. López, V. Agost and M. Barreda	A new C++ Poisson series processor

END OF THE 5th DAY

4 October 2009 SESSION: Computational Methods I CHAIR: S. G. Fountoukis (ROOM 1)		
09:00 – 09:30	P. Herman, D. Zapletal, I. Barvik	Computer Simulation of the Anisotropy of Fluorescence Decay in Ring Molecular Systems with the usage of paralelism: Influence of disorder and ellipticity
09:30 – 10:00	C. Harvey and S. Wang	Modeling Of Delamination Propagation In Composite Laminated Beam Structures
10:00 – 10:30	Zu Soh, Toshio Tsuji, Noboru Takiguchi, Hisao Ohtake	A Neural Network Model for Olfactory Glomerular Activity Prediction
10:30 – 11:00	S. G. Fountoukis and D. T. Chatzistavrou	Pattern Oriented Design of Cluster Running Object Medical Information Systems
Coffee Break		
11:30 – 12:00	H.Aliouat M.Zouikri	Influence of Amino Acid Side Chain Preceding Azaprolyl Residue on β-turn Stabilization
12:00 – 12:30	Qinghua Feng	AGE Method For 2D Hyperbolic Equations

4 October 2009 SESSION: Computational Methods II CHAIR: Ulrike Salzner (ROOM 2)		
09:00 – 09:30	Thomas Punz	
09:30 – 10:00	Ulrike Salzner and Roi Baer	Density Functional Theory Orbital Energies for Predicting Ionization Energies
10:00 – 10:30	Kritsana Sagarik and Charoensak Lao-ngam	Structures and Dynamics of Proton Transfer at Sulfonate Group of Nafion
10:30 – 11:00	İsmail Aslan	Constructing exact and explicit solutions to NDDEs by a discrete version of the (G'/G)-expansion method
Coffee Break		

4 October 2009 SESSION: Computational Methods III CHAIR: Roman Trobec (ROOM 3)		
09:00 – 09:30	Daniela Marinescu, Ioana Manafi (Ramniceanu), Dumitru Marin	On the Slutsky's Equation in Risk and Uncertainty
09:30 – 10:00	Francisco Matorras	CMS Computing Model
10:00 – 10:30	Roman Trobec	Analysis of Errors in MLPG Methods
10:30 – 11:00	Ioana Manafi (Ramniceanu), Daniela Marinescu , Dumitru Marin	The Evolution of The Wage and Effort
Coffee Break		
11:30 – 12:00	V. Prokop and K. Kozel	Numerical solution of non-Newtonian power-law flow through channel and bypass
12:00 – 12:30	Bao-Xing Li , Xiao-Jun Ren, Yi-Feng Xu	Oxidation reactions of H2O and N2O with Si clusters: A first-principles study
12:30 – 13:00	Chen Jingyuan , Jiang Chao, Zha Li and Wang Yuchen	Risk Management of Assets and Liabilities in Commercial Banks Based on Gravity Model

4 October 2009 SESSION: Computational Methods IV CHAIR: M. López (ROOM 4)		
09:00 – 09:30	Chen Jingyuan, Jiang Chao, Zha Li and Wang Yuchen	Risk Management of Assets and Liabilities in Commercial Banks Based on Gravity Model
09:30 – 10:00	C.-O. Hwang	Field-induced Kosterlitz-Thouless transition in critical triangular-lattice antiferromagnets: Yang-Lee zero analysis
10:00 – 10:30	I.S. Kardaras, V.N. Stavrou, I.G. Tsoulos and T.S. Kosmas	Calculations of μ – wavefunctions in mounic atoms using a genetic algorithm
10:30 – 11:00	Jelena Tamuliene	Quantum Mechanical Study On The Fragmentation Of The POPOP Molecule
Coffee Break		
11:30 – 12:00	Naveen Kumar Sharma and Manu Pratap Singh	Performance analysis of pattern classification for the Handwritten English vowels with Back propagation & DG-RBF Feed forward Neural Networks
12:00 – 12:30	A. A. El-Meligi	Experimental Conditions for Intercalation of Organic Compounds into Semiconductor Nanomaterial

4 October 2009 SESSION: Computational Methods V CHAIR: E.B. Dolgusheva (ROOM 5)		
09:00 – 09:30	S.Chitra and C.Shakthivadivoo	Embedding function and Johnson alloy potential for the modelled Mg -Al-Sr ternary alloys
09:30 – 10:00	S.Chitra	Monte Carlo simulation using Johnson potential on Mg-Gd-Y alloy for Debye temperature
10:00 – 10:30	M.R. Eskandari and H. Khajehazad	Calculation of structure parameters for nonsymmetric three body molecules
10:30 – 11:00	E.B. Dolgusheva and V.Yu. Trubitsin	Vibrational Spectra and Anharmonic Effects in Crystals Studied by Molecular Dynamics Simulation
Coffee Break		
11:30 – 12:00	Lyndon N. Smith and Melvyn L. Smith	Analysis of Three Dimensional Textures Through use of Photometric Stereo, Co-occurrence Matrices and Neural Networks
12:00 – 12:30	Jian LEE ,Yuan-hua JIA, Tao YUAN, Jinjin CAO, Yong ZHANG, Wei XU	Correlation Analysis of Traffic Construction Investment and Regional Economy in Typical Province of China
12:30 – 13:00	Alexei A. Stuchebrukhov	Coupled electron and proton transfer in Complex I and Complex IV of the respiratory chain: Insights from computer simulations

4 October 2009 SESSION: Computational Methods VI CHAIR: Alexander Spivak (ROOM 6)		
09:00 – 09:30	Bouzid BOUDJRIBA	Synthesis and characterization of an hybrid material of fluorovanadoaluminophosphate type, templated by 1, 3 diaminopropane
09:30 – 10:00	Alexander Spivak	Successive Approximations for Optimal Control of Nonlinear Time Delay Systems
10:00 – 10:30	Mahboobeh Manoochehri, Reza Fazael, Meghdad Karimi, Mohammad Faridi, Bashir Ahmad Rajabi, Nasir Ahmad Rajabi	Excess Properties of Binary Mixture of Mesitylene and Vinyl acetate at T = (298.15, 303.15 and 308.15) K
10:30 – 11:00		
Coffee Break		

4 October 2009 SESSION: Computational Methods VII CHAIR: Zacharias Anastassi (ROOM 1)		
15:00 – 15:30	Cezary Czaplewski, Artur Giełdon, Krzystof Smalara, Maciej Bobrowski	Molecular dynamics simulation of polymerization of p-xylylene
15:30 – 16:00	M.Z.Tokar	Numerical modeling of transport barrier formation
16:00 – 16:30	León Escobar-Moreira, José Antonino-Daviu, Martin Riera-Guasp	Detection of Broken Rotor Bars in Induction Machines: An Approach Using Wavelet Packets in MCSA
16:30 – 17:00	Aleš Jirk, Josef Brechler	Stratified atmospheric flow modeling
Coffee Break		
17:30 – 18:00	Vladimír Fuka, Josef Brechler	Dispersion of particulate matters past an obstacle – preliminary model results and comparison with experiment
18:00 – 18:30	A.I. Shkrebtii, T. Teatro, L. Henderson, I.M. Kupchak, Z. Ibrahim and F. Gaspari	Temperature dependent vibrational and optical spectroscopy of hydrogen in silicon: from crystalline to amorphous materials

4 October 2009 SESSION: Computational Methods VIII CHAIR: Elena Şendroiu (ROOM 2)		
15:00 – 15:30	Boštjan Drnovšek, Vladimir Bregar	Application of 3D finite-element numerical modeling for the analysis of composite properties
15:30 – 16:00	Elena Şendroiu	Sheaf Construction
16:00 – 16:30	Filip Uhlík, Zdeněk Slanina and Shigeru Nagase	Stabilities in Metallofullerene Series X@C74 and Y@C82
16:30 – 17:00		
Coffee Break		
17:30 – 18:00	Jacek Korchowiec	Elongation cutoff technique at Kohn-Sham level of theory: an efficient sparse matrix algebra approach to linear scaling
18:00 – 18:30	Q.B. Lin, A.Y. Li, Y.H. Wen, Z.Z. Zhu	Magnetism of a free-standing W monoatomic sheet
18:30 – 19:00	LIU Yong-mei, GUAN Yong, ZHANG Jie, WU Min-hua, WU Lin-wei	Application in DSP/FPGA Design of Matlab/Simulink

4 October 2009 SESSION: Computational Methods VIII CHAIR: S. G. Fountoukis (ROOM 3)		
15:00 – 15:30	M.Z.Tokar	Numerical modeling of transport barrier formation
15:30 – 16:00	Jalali Nadooshan Mohammad Reza, Salavati Hossein	Calculation of activation energy and activation enthalpy of kcl:eu by computation methods
16:00 – 16:30	S. G. Fountoukis and I. P. Argyropoulos	Inter Process Communication over Fast Multi Core Cluster Interconnections
16:30 – 17:00	Yongkyu Kwak, Rakwoo Chang, and Yeshitila Gebremichael	Monte Carlo Simulation Studies of Neurofilament Brushes
Coffee Break		
17:30 – 18:00	Eonji Lee, Ji-Hyung Han, Rakwoo Chang, and Taek Dong Chung	Grand-Canonical Monte Carlo Simulation Studies of Polyelectrolyte Diode
18:00 – 18:30	S. G. Fountoukis and I. P. Argyropoulos	Mobile Agent Location in Distributed Environments
18:30 – 19:00	Jumin Lee, Rakwoo Chang, and Yonghwan Kim	Molecular Modeling Studies: Enantioselectivity of Candida Antarctica Lipase B for Lactate Isomers

4 October 2009 SESSION: Computational Methods VIII CHAIR: Wang Jun (ROOM 4)		
15:00 – 15:30	Wang Jun	A three-phase hybrid constitutive model for TiNiNb shape memory alloys
15:30 – 16:00	Yu Shaorong, Xu Bin, Yin Yihui, Tan Yun, Sun Ying	Finite element analysis for a pressure vessel of HR-2 steel
16:00 – 16:30	G. Papakaliatakis and D. Mentou	The influence of the adjacent fibres on debonding arrest of a broken fibre in SiC/Al composites

POSTER SESSION

J. Kromulski, T. Pawlowski, J. Szczepaniak and L. Lowinski	Application of operational modal analysis and operational deflection shapes (ods) on the study of vehicle dynamic
Sylwia Smuczyńska, Piotr Skurski, and Maciej Bobrowski	Reactions of parylenes with double bonds. An ab initio study
A. G. Papadopoulos, N. D. Charistos and M. P. Sigalas	Aromaticity Variation in BN substituted triphenylene. A theoretical study
Paweł Siuda, Joanna Sadlej	Calculations of NMR parameters of methane clathrate hydrates
Jan Szczepaniak and Ryszard Grzechowiak	Modelling Of Agricultural Set (Tractor-Potato Planter) Dynamics In Aspect Of Vehicle Motion Stability And Steerability

4 October 2009
19:10 ***Closing Ceremony***

END OF THE 6th DAY