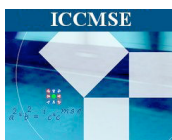


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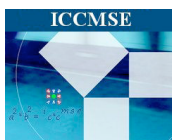
Tuesday 29 September 2009 Kirtman's symposium, SESSION: 1 CHAIR: Michael SPRINGBORG, (ROOM 1)		
09:00 – 09:40	<i>Celso de Melo</i>	A Quantum Chemical Approach to the Molecular Conductance Problem
09:40 – 10:20	<i>Miquel Torrent-Sucarrat</i>	The Applicability of the HSAB Principle
10:20 – 10:40	<i>Feng Long Gu</i>	Band Structure of Polymer Extracted from Oligomer Calculations by Elongation Method and Its Applications to Nanosystems
10:40 – 11:00	<i>Oleksandr Loboda</i>	Efficient algorithm for computing the orbital energies within elongation method
Coffee Break		
11:20 – 12:00	<i>Ajit Thakkar</i>	A hierarchy for additive models of polarizability
12:00 – 12:20	<i>Kikuo Harigaya</i>	Exciton Effects in Optical Absorption Spectra of Boron-Nitride Nanotubes
12:20 – 13:00	<i>Yuriko Aoki</i>	Generalization Elongation Method for Gigantic Systems of 1D, 2D, and 3D
13:00 – 13:20	<i>Violina Tevekeliyska</i>	Implementation of a vector potential method in <i>ab initio</i> Hartree-Fock code
Lunch Break		
Tuesday 29 September 2009 Kirtman's symposium, SESSION: 2 CHAIR: Feng Long GU, (ROOM 1)		
15:00 – 15:20	<i>Roberto Dovesi</i>	Coupled perturbed HF/KS calculation of the



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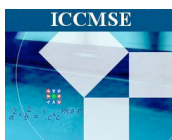
		polarizability of crystalline systems. The case of six members of the garnet family
15:20 – 15:40	<i>Michael Springborg</i>	On the dependence of bulk properties on surfaces
15:40 – 16:00	<i>Edith Botek</i>	Linear and nonlinear second-order susceptibilities of molecular crystals
16:00 – 16:20	<i>Bin Peng</i>	Homoleptic Mononuclear and Binuclear Ruthenium Carbonyls $\text{Ru}(\text{CO})_n$ ($n=3-5$) and $\text{Ru}_2(\text{CO})_n$ ($n=9-6$)
16:20 – 16:40	<i>Yi Dong</i>	Determining the size dependence of structural properties of clusters
16:40 – 17:00	<i>Aggelos Avramopoulos</i>	Non Linear optical properties of rare gas compounds
Coffee Break		
17:20 – 18:00	<i>Mauro Ferrero</i>	The Calculation of the Static First- 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	<i>Heribert Reis</i>	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	<i>Marek Wojcik</i>	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



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Wednesday 30 September 2009 Kirtman's symposium, SESSION: 3 CHAIR: Josep M. LUIS, (ROOM 1)		
09:00 – 09:40	<i>Mark Hoffmann</i>	Generalized Van Vleck Perturbation Theory Study of Chlorine Monoxide
09:40 – 10:20	<i>Roberto Cammi</i>	On two recent developments of the Polarizable Continuum Model: squeezing molecules and correlating their electrons.
10:20 – 10:40	<i>Magdalena Pecul</i>	Environmental Effects on the Raman Optical Activity Spectra of Amino Acids: Theory and Experiment
10:40 – 11:00	<i>Elena Bogdan</i>	Experimental and Theoretical Investigations of Reference Molecules for Nonlinear Optics :The Example of Acetonitrile
Coffee Break		
11:20 – 12:00	<i>Kenneth Ruud</i>	Opening the Property Treasure Chest : a DFT Approach for Calculating Arbitrary Molecular Properties in the Relativistic and Nonrelativistic Domains
12:00 – 12:20	<i>Frédéric Castet</i>	Second-Order Nonlinear Optical Responses of Flexible Pyridine-Pyrimidine Foldamers
12:20 – 12:40	<i>Zhongzhi Yang</i>	Molecular Face Theory (MFT): The Topology Analysis of the (PAEM) and Local descriptors of reactivity mapping on the Molecular Face
12:40 – 13:00	<i>Robert Zalesny</i>	Critical assessment of density functional theory for computing vibrational (hyper)polarizabilities
Lunch Break		



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Wednesday 30 September 2009 Kirtman's symposium, SESSION: 4 CHAIR: Benoît CHAMPAGNE, (ROOM 1)		
15:00 – 15:40	<i>Ove Christiansen</i>	Vibrational Response Theory
15:40 – 16:00	<i>Josep M. Luis</i>	Nonlinear optical properties and large amplitude anharmonic vibrational motions
16:00 – 16:20	<i>Milena Spassova</i>	A DFT Study of the Second Hyperpolarizability of Linear ladder-type O-, N-, S-, and B-Fused Heterocyclic Oligomers
16:20 – 16:40	<i>Ryohei Kishi</i>	Long-Range-Corrected UDFT Study on Second Hyperpolarizabilities of Open-Shell Singlet Systems
16:40 – 17:00	<i>Kalju Kahn</i>	Anharmonic Vibrational Analysis Of Water At CCSD(T) Level: Comparison Of Traditional and Explicitly Correlated Methods
Coffee Break		
17:20 – 18:00	<i>Manthos Papadopoulos</i>	Novel Photonic Materials
18:00 – 18:20	<i>Benoît Champagne</i>	Bernie KIRTMAN in Pictures

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