ICCMSE 2010, Psalidi, Kos, Greece, October 3–8
Methods in Quantum Chemistry
A symposium in honor of
Jiří Čížek and Josef Paldus

04 October 2010 SESSION: Non-Linear Optical Properties of Matter: From Molecules to Condensed Phases CHAIR: Aggelos Avramopoulos (ROOM 7)		
11:05 – 11:35	Ryohei Kishi	Time-Dependent Density Functional Theory Based Quantum Master Equation (DFT-QME) Approach: Calculation and Analysis Methods for Dynamic (Hyper)polarizabilities
11:35-12:05	Evelien De Meulenaere	Prediction of First Hyperpolarizability of Fluorescent Proteins
12:05-12:35	Bernard Bourguignon	The response of molecules bonded to metallic nanoparticles to electronic excitation of the nanoparticles : bond breaking, shape and size effects
12:35-13:05	Tomo-Hayakawa	Structure and Third-order Optical Susceptibility of Divalent Metal Oxide (MO; M=Zn, Mg, Ca, Sr, Ba) doped Nb2O5-TeO2 Glasses
13:05-13:35	Pierre-Francois Brevet	Multipolar Nonlinear Optics of Metallic Nanoparticles
LUNCH BREAK		
CHAIR: Prasanta K Nandi (ROOM 7)		
15:00-15:20	Aggelos Avramopoulos	Designing molecules for NLO applications
15:20-15:40	Maria Helena Garcia	Design and sythesis of NLO Efficient Organometallic Molecules

15:40-16:00	Juan-Ho Choi	Linear and nonlinear spectroscopy of polypeptide:Numerical Simulation studies
16:00-16:30	Prasanta K. Nandi	Structure-Property Correlation Study Through Sum-Over-State Approach
COFFEE BREAK		
05 October 2010 **SESSION: Non-Linear Optical Properties of Matter: From Molecules to Condensed Phases** **CHAIR: Pierre-Francois Brevet** **(ROOM 7)**		
11:05:11:35	Mihai V. Putz	Developing Density Functional Theory for Bose-Einstein Condensates. The Case of Chemical Bonding
11:35 – 11:55	Tateki Ishida	Theoretical Investigation of Polarization Effects in Solution: Importance of Solvent Collective Motions
11:55-12:25	Ji Wei	Spherical or cubic,which shape is better?A systematic investigation into size and shape-dependent multi-photon absorption in semiconductor nanocrystals
12:25-12:45	Mathias Hanauer	Calculation of response properties with explicitly correlated coupled-cluster methods
12:45-13:05	Hideaki Shirota	Intermolecular Dynamics in Liquids Studied by A Third-Order Nonlinear Spectroscopy

Design and Synthesis of NLO Efficient Organometallic Molecules

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Abstract. Second-order nonlinear optical (SO-NLO) properties of group 8 half-sandwich organometallic complexes have been intensively studied throughout the last 15 years, making this class of compounds relevant for the continuous search of NLO materials. This contribution surveys the ongoing efforts to design, characterize and optimize the NLO properties of this class of compounds. Computational studies, namely DFT calculations, were performed for several model molecules in order to predict the first hyperpolarizabilities and to support experimental evidences.

Keywords: Non-linear optics; first hyperpolarizability β.organometallics; half-sandwich complexes; ruthenium (II); iron(II);
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