

ELECTRON CORRELATION FOR THE WHOLE PERIODIC TABLE
A theoretical chemistry Symposium in honour of Björn Roos
Crete, October 27-29 2006

October 27, 2006

Schedule	Speaker	Title of contribution
09.00 - 09.10	Laura Gagliardi, Geneva, Switzerland	<i>OPENING</i>
09.10 - 09.40	Rudy Marcus, Caltech, Pasadena, USA	<i>Enzymatic catalysis : experiments, theory and computations, open questions and a unified view</i>
09.40 - 10.10	Peter Taylor, Warwick, Coventry, UK	<i>How do we treat electron correlation in small carbon rings ?</i>
10.10 - 10.40	Cristina Puzzarini, Bologna, Italy	<i>How accurately can structural, spectroscopic and thermochemical properties be predicted by ab initio computations ?</i>
10.40 - 11.10	COFFEE BREAK	
11.10 - 11.40	Ursula Roethlisberger, Lausanne, Switzerland	<i>Dispersion-Corrected Density Functional Calculations</i>
11.40 - 12.10	Kristine Pierloot, Leuven, Belgium	<i>Theoretical modeling of the relative spin-state energetics in transition-metal compounds : how accurate is CASPT2 ?</i>
12.10 - 12.40	Jun-ya Hasegawa, Kyoto, Japan	<i>Photobiology and biospectroscopy studied by SAC-CI method</i>
LUNCH		
16.00 - 16.30	Margareta Bloomberg, Stockholm, Sweden	<i>Modelling reactions of cytochrome c oxidase : Proton pumping and reduction of molecular oxygen and nitric oxide</i>
16.30 - 17.00	Marco Garavelli, Bologna, Italy	<i>Spectral tuning and photochemical reactivity control in biological chromophores : towards an accurate computational photobiology</i>
17.00 - 17.30	COFFEE BREAK	
17.30 - 18.00	Spiridoula Matsika, Temple, Philadelphia, USA	<i>Electronically excited states and conical intersections of complex systems using high level ab initio methods</i>
18.00 - 18.30	Roland Lindh, Lund, Sweden	<i>Cholesky decomposition of the two-electron integrals : A reliable tool for linear scaling methods ?</i>

October 28, 2006

Schedule	Speaker	Title of contribution
09.00 - 09.30	Michael Haeven, Emory, Atlanta, USA	<i>Probing actinide electronic structure using fluorescence and multi-photon ionization spectroscopy</i>
09.30 - 10.00	Valérie Vallet, Lille, France	<i>The importance of electron correlation and intermediate coupling in the spectroscopy of actinide molecules</i>
10.00 - 10.30	Pekka Pyykkö, Helsinki, Finland	<i>News on heavy-element chemistry</i>
10.30 - 11.00	COFFEE BREAK	
11.00 - 11.30	Luis Serrano, Valencia, Spain	<i>DNA nucleobases photoreactivity : "The role of quantum chemistry in modern photochemistry</i>
11.30 - 12.00	Christel Marian, Düsseldorf, Germany	<i>Vibronic spin-orbit coupling: a clue to intersystem crossing in psoralen</i>
12.00 - 12.30	Luis Seijo, Madrid, Spain	<i>Ab initio calculations on lanthanide and actinide ions in solids using MOLCAS</i>
LUNCH		
15.30 - 16.00	Gernot Frenking, Marburg, Germany	<i>Multiple bonds in heavy atom molecules : To be or not to be, that is the question</i>
16.00 - 16.30	Chantal Daniel, Strasbourg, France	<i>From small organometallics to large metal-to-ligand-charge-transfer complexes : excited states quantum chemistry</i>
16.30 - 17.00	COFFEE BREAK	
17.00 - 17.30	Odile Eisenstein, Montpellier, France	<i>Organometallic reactivity from a computational point of view : some recent examples</i>
17.30 - 18.00	Mike Hall, Texas A&M, Texas, USA	<i>Modeling metalloenzymes : Nickel-iron and di-iron hydrogenases</i>
18.00 - 18.30	Jennifer C. Green, Oxford, UK	<i>Accessing two final states by ionizing the f electron in a Ce(III) compound</i>
21.00-23.00	Poster Session	

October 29, 2006

Schedule	Speaker	Title of contribution
09.00 - 09.30	Trygve Helgaker, Oslo, Norway	<i>Self-consistent filed methods applied to large molecular systems</i>
09.30 - 10.00	Tomasz Wesolowski, Geneva, Switzerland	<i>Eliminating orbitals from quantum mechanical description of many-electron systems : A step beyond Kohn-Sham</i>
10.00 - 10.30	Kimihiko Hirao, Tokyo, Japan	<i>Photoelectron spectra of $Re(CO)_5X$ ($X=Cl, Br, and I$): CASPT2, SAC-CI, and DFT study</i>
10.30 - 11.00	COFFEE BREAK	
11.00 - 11.30	Antonio Rizzo, Pisa, Italy	<i>Non linear optical properties of chiral molecules</i>
11.30 - 12.00	Jeppe Olsen, Aarhus, Denmark	<i>Bridging the gap between multi-reference perturbation and coupled cluster methods</i>
12.00 - 12.30	Henry F. III Schaefer, Athens, USA	<i>Lesions in DNA subunits : Foundational studies of structures and energetics</i>
12.30 - 12.40	Henry F. III Schaefer, Athens, USA	<i>Concluding remarks</i>
LUNCH		