

**9-th Central European Symposium on Theoretical Chemistry
CESTC 2010**

Nový Smokovec, Slovakia, September 12 - 15

Preliminary programme

Sunday, September 12

15:00-17:00 ***Registration***

Chairman: Miroslav Urban

17:00-17:10 ***Opening***

17:10-17:55 Josef Michl

Trying to Understand the Mysterious Fluorescence of σ Systems: Oligosilanes

17:55-18:40 Andras Stirling

Reaction mechanism from quantum chemistry: unbiased and biased simulations

18:40-19:25 Florent Louis

Thermochemical data calculation by quantum chemistry methods: application to ten species involved in low-temperature oxidation mechanism of o-xylene

19:30-21:00 ***Welcome Party***

Monday, September 13

Chairman: Stanislaw Kucharski

- 8:30-9:15 Piotr Piecuch
Local correlation coupled-cluster methods exploiting cluster-in-molecule ansatz and their multi-level generalizations
- 9:15-9:35 Tatiana Korona
Local treatment of electron correlation for first-order molecular properties from expectation-value CCSD theory
- 9:35-9:55 Tamás Zoboki
Electron Correlation Calculations with Strictly Localized Orbitals
- 9:55-10:15 Kalju Kahn
Anharmonic Vibrational Analysis with Explicitly Correlated Wavefunctions
- 10:15-10:45 **Coffee Break**

Chairman: Peter Surjan

- 10:45-11:30 Agnes Nagy
Pair density functional theory
- 11:30-11:50 Alexei Arbuznikov
Local hybrids: conceptually simple hyper-GGA exchange-correlation functionals for the Kohn-Sham density functional calculation of a wide range of properties
- 11:50-12:10 Dorota Rutkowska-Zbik
DFT Studies on Catalytic Oxidation of Cyclohexene on Manganese Porphyrins
- 12:10-12:30 Prokopis Andrikopoulos
Periodic-DFT study of the N₂O decomposition over Fe-ferrierite
- 12:30-14:00 **Lunch**

Chairman: Philippe Durand

- 14:30-15:15 Katarzyna Pernal
Treating static and dynamic correlation with range-separated density and density matrix functionals
- 15:15-15:35 Michal Przybytek
Gaussian and Finite-Element method for the calculation of Coulomb integrals
- 15:35-15:55 Štefan Varga
The Brillouin zone integration problem in density fitting of extended systems
- 15:55-16:25 **Coffee Break**

Chairman: Bogumil Jeziorski

- 16:25-16:45 Dariusz Kedziera
Wave function in the relativistic two component methods
- 16:45-17:05 Konrad Piszczatowski
Relativistic, QED and nonadiabatic effects in the interaction of hydrogen atoms
- 17:05-17:25 Ágnes Szabados
The problem of small coefficients in SS-MRPT
- 17:25-17:45 Péter Szakács
Jahn-Teller distortion and zero-field-splitting in carbon nanotubes
- 17:45-18:05 Libor Veis
Quantum chemical computations on quantum computers
- 18:30-20:00 **Dinner**
- 20:00-21:30 **Posters 1**
pp 64-101 (see Book of Abstracts)

Tuesday, September 14

Chairman: Stanislav Biskupič

- 8:30-9:15 Roman Čurík
Message to quantum chemists: What we learned about DFT by modelling electron-molecule collisions
- 9:15-9:35 Petr Čársky
Prospects of using MP2 for electron scattering
- 9:35-9:55 Lubomír Skála
Quantum mechanics and mathematical statistics
- 9:55-10:15 Ján Šimunek
Orbital Optimized Second-Order Many-Body Perturbation Theory Via Coupled Cluster Ansatz
- 10:15-10:45 **Coffee Break**

Chairman: Jan Hrušák

- 10:45-11:30 Thomas Hofer
Characterisation of anisotropic hydration phenomena with QM/MM models
- 11:30-11:50 Mariusz Paweł Mitoraj
A Combined Charge and Energy Decomposition Scheme for Analysis of Chemical Bonds and Reaction Paths
- 11:50-12:10 Łukasz Piękoś
Molecular dynamics modeling of half-metallocene titanium(IV) ethylene polymerization catalysts
- 12:10-12:30 Aleš Vítek
Structural changes in the water tetramer and hexamer. A Combined Monte Carlo and DFT study.
- 12:30-14:00 **Lunch**

Chairman: Alexander Sax

- 14:30-15:15 Christoph Flamm
In silico Evolution of Early Metabolism
- 15:15-15:35 Ivana Paidarova
Kinetic equations and dissipation.
- 15:35-15:55 Katarzyna Kulczycka
Internal flexibility of clindamycin
- 15:55-16:25 **Coffee Break**
- 16:30-18:00 **Posters 2**
pp 103-145 (see Book of Abstracts)
- 19:00-21:30 **Conference Dinner**

Wednesday, September 15

Chairman: Ivan Černušák

- 8:30-9:15 Miroslav Medved
Study and design of nonlinear optical materials: from molecules, through oligomers to polymers
- 9:15-9:35 Laszlo Nyulaszi
Some predictions on stable molecules: failure and success.
- 9:35-9:55 Dana Nachtigallova
Photodynamics of pyrimidine-based molecules: Effect of substitution and initial energy
- 9:55-10:25 **Coffee Break**

Chairman: Jiří Pittner

- 10:25-11:10 Monika Musial
Fock space coupled cluster theory for two-valence sectors
- 11:10-11:30 Kiran Bhaskaran Nair
Multireference State-Specific Mukherjee's Coupled Cluster Methods With Triexcitations
- 11:30-11:50 Istvan Mayer
The promotion energy of an atom in a molecule
- 11:50-12:10 Leszek Meissner
An extension of the coupled-cluster corrected configuration interaction method
- 12:10-12:20 **Closing**
- 12:30-14:00 **Lunch**