

First Czech-Japan Theoretical Chemistry Symposium
September 14 – 16, 2005
Institute of Organic Chemistry and Biochemistry (IOCB),
Academy of Sciences of the Czech Republic, in Praha

September 14

Opening



Prof. Hiroshi Nakatsuji
(Kyoto University)



Prof. Zdenek Havlas
(IOCB)

Oral Presentations



Prof. Masahiko Hada
(Tokyo Metropolitan University)
“NMR Chemical Shifts of Metal Complexes in
Copper Enzymes and Heme Proteins”



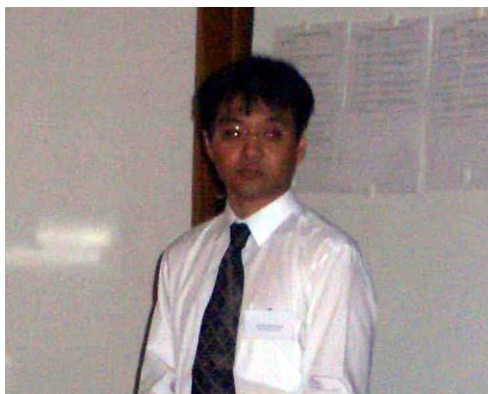
Prof. Hiromi Nakai
(Waseda University)
“Energy Density Analysis”



Dr. Jun-ya Hasegawa
(Kyoto University)
“Excited States and Electron Transfer in Bacterial
Photosynthetic Reaction Center: SAC-CI Study”



Dr. Georg Pruemper and Prof. Kiyoshi Ueda
(Tohoku University)
“High resolution molecular core-level
photoelectron spectroscopy”



Dr. Masahiro Ehara
(Kyoto University)
“Theoretical Fine Spectroscopy: vibrational
spectra and excited-state structures”



Dr. Dana Nachtigallova

(IOCB)

“Theoretical Study of Excited States of H-bonded and Stacked DNA Base Pairs”



Prof. Shigeki Kato

(Kyoto University)

“Free energy surfaces of photochemical processes in solution”



Dr. Jiri Cerny

(IOCB)

“Theoretical Description of Keto-Enol Equilibrium of 7- and 9- methylguanines in their ground and excited states”



Dr. Eva Mrazkova

(IOCB)

“Excited States of HCN and H₂O...HCN Systems: Photoacidity and Dynamics of Proton Transfer”

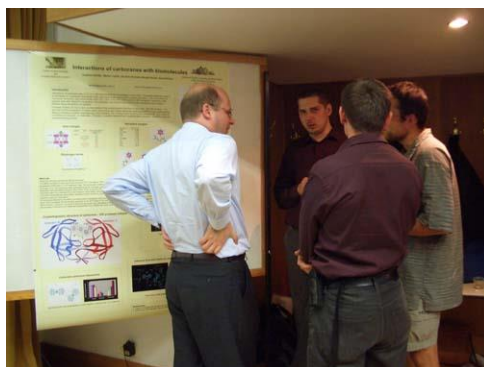


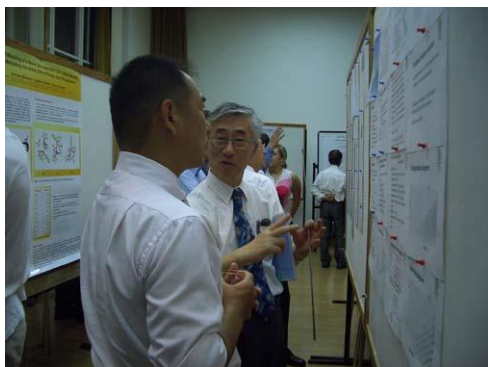
Prof. Pavel Hobza

(IOCB)

“Why Evolution Selected the Watson Crick Binding Motif in Guanine...Cytosine Base Pair: Experimental and Theoretical Study in the Ground and Excited States”

Poster Presentations





September 15
Oral Presentations



Prof. Shigeyoshi Sakaki
(Kyoto University)
“Theoretical Study of Catalytic Reactions by Transition
Metal Complexes”



Dr. Ondrej Demel
(Heyrovsky Institute)
“Multireference Brillouin-Wigner Coupled Cluster
Method with Triexcitations: Iterative and Noniterative
Approach”



Dr. Mitsutaka Okumura
(Osaka University)
“Material Oriented Quantum Chemistry: Hybrid DFT
calculation of mesoscopic radical clusters”



Dr. Stepan Sklenak
(Heyrovsky Institute)
“Comparative Ab Initio and DFT Study of CuNO_2 and
 $\text{Cu}+\text{NO}_2$ ”



Dr. Kazuo Toyota
(Osaka City University)
“Calculation of zero field splitting in organic molecules
using the unrestricted Hartree-Fock molecular orbitals”



Prof. Jiri Pittner
(Heyrovsky Institute)
“New Developments in the Multireference Brillouin-
Wigner Coupled Cluster Method”



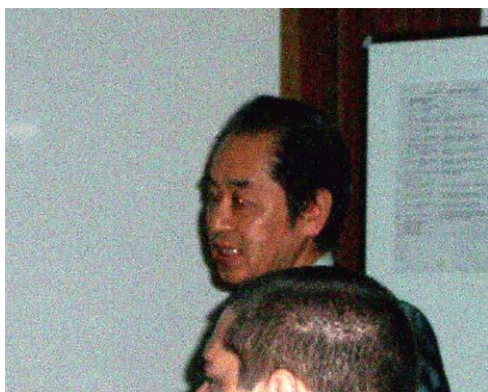
Prof. Petr Carsky

(Heyrovsky Institute)

“Vibrational Excitation by Electron Impact: Need for a Better Exploitation of Expertise Accumulated in Quantum Chemistry”

September 16

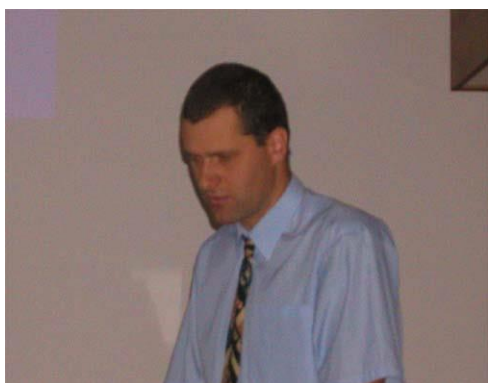
Oral Presentations



Prof. Takeji Takui

(Osaka City University)

“An RDM Approach to the Fine-Structure Tensors of 3-Dimensionally Spin Delocalized Systems: Application to Fullerene C₆₀ and C₇₀ in the High Spin States”



Dr. Lubomir Rulisek

(IOCB)

“Can we think of [n] helicenes as of the potential nanodevices? A theoretical study of the convergence of their physico-chemical properties”



Dr. Hirohiko Kono

(Tohoku University)

“Ultrafast electronic dynamics induced by intense laser fields: from molecules to living cells”



Dr. Jiri Vondrasek

(IOCB)

“Correlated ab initio quantum chemical calculations of stabilization inside hydrophobic core of proteins”



Dr. Shinji Saito

(Nagoya University)

“Dynamics of liquid water and nonlinear two-dimensional Raman spectroscopy”



Prof. Zdenek Havlas

(IOCB)

“Relativistic effects in organic biradicals”



Prof. Iwao Ohmine
(Nagoya University)
“Water Dynamics; fluctuation, phase transition and reactions”



Prof. Koichi Yamashita
(University of Tokyo)
“A non-equilibrium Green's function approach to photoinduced reactions on metal surfaces”



Closing Remarks



Prof. Hiroshi Nakatsuji
(Kyoto University)



Prof. Zdenek Havlas
(IOCB)

For the second Japan-Czech Theoretical Chemistry Symposium in Japan



Prof. Shigeki Kato, Prof. Hiroshi Nakatsuji
(Kyoto University)



Prof. Shigeki Kato, Prof. Shigeyoshi Sakaki, Prof.
Hiroshi Nakatsuji
(Kyoto University)