



## 2<sup>nd</sup> Prague-Vienna Quantum Chemical Seminar

Institute of Organic Chemistry and Biochemistry AS CR, v.v.i., Prague,  
June 23-24, 2009

**Venue:** Villa Lanna, V Sadech 1, Prague 6  
Fleming Square 2, Prague 6, IOCB club

### Program

<b>June 23, 2009</b>		
14:00	R. Zahradník	Opening
Chair: P. Hobza		
14:15	V. Bonačić-Koutecký	Theoretical methods for analysis and control of nonadiabatic dynamics in complex systems
15:00	M. Ruckebauer	QM/MM in Photodynamics
15:25	J. Szymczak	Why thymine has the longest lifetime of all nucleobases
15:50	F. Plasser	Electronic coupling in the ethylene dimer cation
16:15		Coffee Break
Chair: M. Pitoňák		
16:45	N. Kungwan	Excited-state proton transfer of 2,(2'-hydroxyphenyl)benzothiazole in water cluster: a TDDFT molecular dynamics study
17:10	B. Sellner	Reaction pathways with COLUMBUS: The MEP program package
17:35	H. Pašalić	Interactions of soil constituents: Acetic acid dimer in various environments

18:00	R. Šolc	Theoretical study of electro-optical properties of pi-conjugated systems
18:25		End of Session

**June 24, 2009**

Chair: H. Lischka

9:00	T. Schultz	Excited state spectroscopy of DNA bases: what we can and cannot do
9:45	H.-H. Ritze	Tunneling-induced decay of metastable excited states in model DNA bases
10:30		Coffe Break
Chair: M. Barbatti		
11:00	M. Pitoňák	Nonadditivity of interactions in DNA
11:25	M. Kolář	Does DNA need dispersion?
11:50	V. Špirko	Morphing ab initio surfaces: Beryllium dimer caught in the act of bonding
12:15	A. J. A. Aquino	The charge-transfer states in stacked DNA bases
12:40	D. Nachtigallová	Effect of substituents on excited states of pyrimidine-type molecules
13:05		End of Meeting