



## 1<sup>st</sup> Prague-Vienna Quantum Chemical Seminar

Institute for Theoretical Chemistry, Faculty of Chemistry, University of Vienna  
May 19-20, 2008

**Venue:** Währingerstraße 17, A-1090 Vienna, seminar room, ground floor

### Program

May 19, 2008		
15:00	H. Lischka	Opening
Chair: Adelia Aquino		
15:15	P. Hobza	Benchmark QM Calculations on DNA Base Pairs and Oligopeptides
15:45	K. Riley	Computational Treatment of pi-bonding Systems: How well can we describe Geometries
16:15	J. Rezac	On-the-fly ab initio MD Simulations of Complex Molecular Systems
16:45		Coffee Break
17:15	M. Pitonak	High-accuracy Calculations on Non-covalent Complexes
17:45	D. Nachtigallova	Electronic Splitting in the Excited States of DNA base Homodimers and -trimers: an evaluation of Short-range and Coulombic Interactions
18:15		End of Session

**May 20, 2008**

Chair: Dana Nachtigallova

9:00	M. Barbatti	Exploring conical intersections in heterocycles using mixed quantum-classical dynamics simulations
9:30	M. Ruckebauer	Hybrid multiple-method gradients and their application to dynamics
10:00	J. Szymczak	The microsolvation of aminopyrimidine in the excited state
10:30		Coffee Break
11:00	B. Sellner	CH dissociation in ethylene: the MRCI description of the $\pi\sigma^*$ state
11:30	F. Plasser	Excited-state double proton transfer in [2,2'-bipyridyl]-3,3'-diol – dynamics simulation vs. experiment
12:00	H. Pasalic	Complexation Energies of Hydrogen-bonded Systems in Solution - A Density Functional and Molecular Mechanics Study)
12:20	A. Aquino	Modeling Humic Substances
12:40		End of Meeting