

Hotel Info:

The conference hotel is the Hotel Atlanta located at:
Währinger Str. 33
A-1090 Vienna

Workshop Location:

The Workshop will take place at the faculty of Computer Science of the University of Vienna. The building is located in Währinger Str. 29, next to the hotel. All talks and contributions will be held in seminar room 7 (SR7), which is located on the 1st floor of the building. Track B of the hands-on session will take place in seminar room 8 (SR8), next to SR7.

Lunch Breaks

On Thursday and Friday, lunch will be served at:
Restaurant Königshofer
Beethovengasse 2
A-1090 Vienna

Excursion:

There will be an organized visit to Schlumberger Sparkling Wine Cellars (including tour and tasting) on Friday evening.

The Schlumberger Cellars are located at:
Heiligenstädter Str. 39
A-1190 Vienna
Tram 37, tram stop Guneschgasse or tram D, tram stop Radelmayergasse

Conference Dinner:

The Conference Dinner will take place on Friday at
Heuriger Schübel-Auer
Kahlenberger Str. 22
A-1190 Vienna
Tram D, tram stop Nußdorf Beethovengang
(2nd Entrance close to tram stop: Zahnradbahnstraße 17)



4th Molcas Developers' Workshop

March 30th – April 1st 2016

University of Vienna, Austria



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Wednesday, 30th March 2016

Hands-on Day	SR 7 and SR 8	12.40 – 18.00
12:40	Welcome, Sandwiches	
13:00	Network Setup, General Issues	
14:00	Hands-on Part 1	
15:00	Coffee Break	
15:30	Hands-on Part 2	

Thursday, 31st March 2016

Session 1	SR 7	Chair: Leticia González
9:00	Leticia González Opening	
9:10	Roland Lindh Welcome and Introduction	
9:20	Introduction of Newcomers	
9:40	Markus Reiher Current status of DMRG in Molcas	
10:00	Quan Phung DMRG-CASPT2 Applied for Spin-State Energetics of Metal-Oxo Porphyrins: Does it Work?	
10:20	Andrew Sand Recent Advancements in Multiconfigurational Pair-Density Functional Theory	
10:40	Coffee Break	
Session 2	Chair: Per Åke Malmqvist	
11:00	Michael Odelius Scientific Perspective: Time-Resolved X-ray Spectroscopy and Time-Resolved Photoelectron Spectroscopy	

11:40	Lasse Sørensen Origin Independent Intensities in X-Ray Spectroscopy
12:00	Giovanni Li Manni Combining FCIQMC and CAS Strategies to Circumvent the Exponential Scaling in CASSCF Calculations
12:20	Dongxia Ma Combining Hubbard Model and FCIQMC Methods for Solid State Studies
12:40	Lunch Break at Königshofer
Session 3	Chair: Thomas Bondo Pedersen
14:10	Sam Stoneburner Molcas Implementation of SplitGAS, a Method for Strongly Correlated Systems
14:30	Javier Segarra Marti Nonlinear Bidimensional Spectroscopy Based on Frozen Natural Orbital PT2 Approaches with MOLCAS
14:50	Patrick Zobel CASPT2 - the IPEA Dilemma
15:10	Coffee Break/Poster Session
15:40	Valera Veryazov Licensing of the Codes Developed in Molcas & Discussions

Friday, 1st April 2016

Session 4	Chair: Per-Olof Widmark
9:00	Liviu Ungur Application of MOLCAS for the Investigation of Low-Lying Electronic Structure and Magnetism of Mono- and Poly-Nuclear Lanthanide Compounds
9:20	Steven Vancouillie Interfacing with Molcas through HDF5 and Python
9:40	Felix Plasser Extended Wavefunction Analysis for Multireference Methods
10:00	Ignacio Fernández Galván Nonadiabatic Couplings and Conical Intersections
10:20	Miquel Huix Rotllant Normal Mode Analysis at the CASPT2 Level
10:40	Coffee Break

Session 5	Chair: Markus Reiher
11:00	Sason Shaik Scientific Perspective: A Theory for Bioinorganic Chemical Reactions: Can Multireference and Multiconfiguration Method Contribute?
11:40	Jose M. Hermida Solvated Electron in Water. A Highly Coupled System for a QM/MM Method
12:10	Michael Böckers General Overview on the DFT/Embedding Code
12:20	Luca De Vico LH2 Bacteriochlorophylls Excitation Energies: Pushing the Envelope
12:40	Lunch Break at Königshofer
Session 5	Chair: Nicolas Ferré
14:10	Alessio Valentini Semiclassical Molecular Dynamics in MOLCAS
14:30	Igor Schapiro A Surface Hopping Algorithm for Nonadiabatic Minimum Energy Path Calculations
14:50	Gerrit Groenhof Observe while it Happens: Catching Photobiology in the Act with Computer Simulations
15:10	Coffee Break/Poster Session
15:40	Valera Veryazov and Steven Vancouillie Open Discussion: Dos and Don'ts in Parallel Programming in Molcas
16:50	Roland Lindh Closing Remarks

Social Events

17:30	Departure for Tour of Schlumberger Sparkling Wine Cellars
20:00	Conference Dinner at Heuriger Schübel-Auer