

## Molcas Developers Workshop 2013 - January 29 - 31, 2013 - Zurich / Switzerland ETH Zurich, Campus Science City Hönggerberg, Lecture Hall HCI J 3

Molcas Developers  
Workshop 2013 - January  
29 - 31, 2013 - Zurich /  
Switzerland ETH Zurich,  
Campus Science City  
Hönggerberg, Lecture  
Hall HCI J 3

Location and Travel

Accommodation

Participants

Tuesday, January 29, 2013		
11:00	welcome and introduction by <b>R. Lindh</b>	
12:15	begin of first set of 15 min talks	<b>P.-Å. Malmqvist</b> , Current and future development on the RASSCF/ RASPT2, and RASSI trojka <b>S. Gusarov</b> and <b>A. Kovalenko</b> , Using Koopmans' approximation to calculate the correlation in CASSCF <b>S. Vancoillie</b> , Computational resource limits when performing RASSCF and RASPT2 on large and complex systems <b>V. Veryazov</b> , Multiconfigurational treatment of 2D/3D systems <b>G. Li Manni</b> , GASSCF, GASPT2 and SplitCAS developments in the RASSCF and CASPT2 domain of Molcas
13:30	coffee break with sandwiches	
13:45	2nd set of 15 min talks	<b>F. Aquilante</b> , Development of combined WFT/DFT strategies in Molcas <b>J. Neugebauer</b> , Subsystem DFT for Ground and Excited States <b>L. Seijo</b> , Embedded clusters and orbital mosaics <b>D. Peng</b> , Relativistic exact decoupling methods and their local variants <b>L. Chibotaru</b> , Ab initio calculation of magnetic properties of of anisotropic complexes
15:00	coffee break	
15:15	3rd set of 15min talks	<b>T. Bondo Pedersen</b> , Cholesky decomposition and density fitting in Molcas <b>M. Delcey</b> , CD-CASSCF gradients and non-adiabatic coupling : towards fast non-adiabatic simulations in MOLCAS <b>L. Ungur</b> , Fragment CASSCF calculations and ab initio based simulations of anisotropic exchange interactions in polynuclear complexes <b>P.-O. Widmark</b> , Toolboxes in Molcas <b>V. Vysotskiy</b> , Adaptation of MOLCAS to modern hardware
16:30	coffee break	
16:45	4th set of 15min talks	<b>I. F. Galván</b> , ASEP/MD: a mean field QM/MM method using Molcas and Gromacs <b>F. Melaccio</b> , Getting ready for Molcas/GROMACS QM/MM: automatic preparation of models with GROMACS <b>N. Ferre</b> , QM/MM integration of a polarizable forcefield using ESPF <b>A. Kovalenko</b> and <b>S. Gusarov</b> , Prospective of implementing statistical-mechanical 3D-RISM-KH molecular theory of solvation in MOLCAS
17:45	coffee break	
18:00	last set of 15min talks	<b>I. Schapiro</b> , Surface hopping algorithm for molecular dynamics and the static (MEP and IRC) simulations <b>A. Valentini</b> , New implementations in MOLCAS for nonadiabatic dynamics <b>E. Valeev</b> , Explicitly Correlated Multireference Methods in MOLCAS <b>R. Shepard</b> , The Multifacet Graphically Contracted Function Method <b>M. Pitonak</b> , Cholesky decomposition based coupled-clusters methods in MOLCAS
19:15	free evening	



<b>Wednesday, January 30, 2013</b>		
	Purpose: make the developers guide the MOLCAS project in the strategically correct direction	
09:00 - 12:00	SWOT analysis on the MOLCAS project ( <a href="http://en.wikipedia.org/wiki/SWOT_analysis">http://en.wikipedia.org/wiki/SWOT_analysis</a> )  10:10 - 10:40 coffee break	<b>Agenda:</b> - initiation talk by <b>M. Olivucci</b> : "What shall we do to better tackle problems in photochemistry and photobiology ?" (15 min) - define small working groups - SWOT analysis within these groups - presentation of the groups - final discussion (chaired by <b>R. Lindh &amp; M. Reiher</b> ) Lecture Halls <b>J3, J4, J6, J7</b>
12:00 - 13:30	lunch break	
13:30 - 16:30	group discussions on the MOLCAS development environment	<b>Agenda:</b> - <b>V. Veryazov</b> : "The Molcas Environment" (15 min) - analysis of unique features of Molcas (past, present, future) within the groups (60 min) - presentation of the groups (45 min) - final discussion (60 min) (chaired by <b>R. Lindh &amp; M. Reiher</b> )  coffee will be provided
17:00 - 18:30	break	(preparations for next day by <b>R. Lindh &amp; M. Reiher</b> )
19:00	Dinner	Tessin Grotto ( <a href="http://www.tessin-grotto.ch/">http://www.tessin-grotto.ch/</a> )
<b>Thursday, January 31, 2013</b>		
09:00	wrap-up session ( <b>R. Lindh &amp; M. Reiher</b> )	<b>Agenda:</b> - summary of conclusions on future directions of Molcas development - discuss/find organizer for next Molcas developers' workshop
11:30	closure	



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Participants

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