

MOLCAS WORKSHOP

22-25.07.2013, Wrocław

TEACHER - FRANCESCO AQUILANTE



Dr Francesco Aquilante is an Assistant Professor in Theoretical Chemistry at the Department of Chemistry, Uppsala University in Sweden. Co-author of the MOLCAS-7 quantum chemistry software. His scientific expertise pertains the development of reduced-scaling techniques in the framework of standard quantum chemical methods. More specifically, he has given a decisive contribution in the Cholesky decomposition-based technology. The whole set of recent development in this area of research, as well as a number of insights in the nearby area of density fitting has seen important contribution from his work. Moreover, he has formulated a new methods for orbital localization, essential ingredient of most linear scaling correlated methods. More recently, he has also contributed to the development of novel approaches to the problem of strong electron correlation and multiscale techniques based on quantum mechanical embedding formalism.

PROGRAM

- Monday (22.07.2013): "Ab initio single-reference wavefunction theory"
- Tuesday (23.07.2013): "Multiconfigurational methods (selection of the active space)"
- Wednesday (24.07.2013): "Properties calculations & Bring your case"
- Thursday(25.07.2013): "MOLCAS as a development platform & Cholesky decomposition"

10³⁰ – 13³⁰
Theory & Exercises

13³⁰ – 15⁰⁰
Lunch break

15⁰⁰ – 17⁰⁰
Exercises

GOAL

The purpose of this workshop is to provide problem-solving skills in electronic structure theory. In particular, towards computational methods of desirable accuracy (e.g. those based on the multiconfigurational paradigm) that are not so widespread, due to their 'non black-box' nature when setting up the calculations. Together with the necessary theory, this course includes an overview of the capabilities of the MOLCAS quantum chemistry software.



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PRACTICAL INFORMATION

- * Workshop is free of charge
- * English is the working language
- * Computer access is provided
- * Number of participants is limited
- * The workshop will take place at the Wrocław University of Technology, Janiszewskiego street 11/17, building C-3, room 125

REGISTRATION

To register for the workshop please send an e-mail at the following adress:

molcas.workshop@wcss.pl

title: Molcas Workshop

content: Name, Surname, University
Registration is open until July 17.

Local organizers:

Wojciech Bartkowiak
Agnieszka Roztoczyńska
Justyna Kozłowska
Wrocław Center for Networking
and Supercomputing

* It is also possible to participate in the workshop through the Internet with use of web browser. Please give the information in the registration e-mail if you want to remote participate.