



Centrum Studiów Zaawansowanych Politechniki Warszawskiej  
Center for Advanced Studies Warsaw University of Technology



PROGRAM ROZWOJOWY  
POLITECHNIKI WARSZAWSKIEJ

WARSAW UNIVERSITY OF TECHNOLOGY DEVELOPMENT PROGRAMME

Human - best investment

## CAS VISITING LECTURES SERIES

*Center for Advanced Studies WUT  
invites to the series of „CAS visiting lectures 2013”*

**Dr. Celia Fonseca Guerra &  
Prof. F. Matthias Bickelhaupt**

Department of Theoretical Chemistry, Vrije Universiteit, the Netherlands  
present the

### COURSE ON THE AMSTERDAM DENSITY FUNCTIONAL PROGRAM

23 September 2013

Introduction: Quantum Chemistry and ADF /lec.

Tutorial, Basis sets and Molecular Orbitals /lab.

24 September 2013

From hydrogen atom to Hartree-Fock /lec.

Tautomerization and rotation barriers in gas phase and solvents /lab.

25 September 2013

From Hartree-Fock to DFT /lec.

Choosing a functional in DFT calculations and SN2 Reaction Profiles/lab.

26 September 2013

Kohn-Sham MO Theory /lec.

Energy decomposition analyses and MO interaction diagrams /lab.

The **lectures** will take place between 11:15-1:00, Audytorium Zawadzkiego,  
the Chemistry Building / Noakowskiego Street 3, Warsaw

The **laboratories** will take place between 2:15-5:00, lecture hall no. 130,  
the Chemical Technology Building / Koszykowa Street 75, Warsaw

For more detailed information please visit the websites:  
[www.csz.pw.edu.pl](http://www.csz.pw.edu.pl)  
[http://konwersatorium.pw.edu.pl/oferta/v\\_lectures.html](http://konwersatorium.pw.edu.pl/oferta/v_lectures.html)



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