REGIONÁLNÍ CENTRUM POKROČILÝCH TECHNOLOGIÍ A MATERIÁLŮ
Regional Centre of Advanced Technologies and Materials

EVROPSKÁ UNIE
EVROPSKÝ FOND PRO REGIONÁLNÍ ROZVOJ
INVESTICE DO VAŠÍ BUDOUCNOSTI

2007–13
OP Výzkum a vývoj pro inovace

Seminář RCPTM – Ing. Matúš Dubecký, Ph.D.

Přednášející: Ing. Matúš Dubecký, Ph.D., Institute of Physics and Institute of Electrical Engineering, Slovak Academy of Sciences, Bratislava, Slovakia

Termín a místo konání semináře: čtvrtek 19.7. 2012 v 15.00 hod v učebně LP 3.005

Název přednášky: Molecular Electronic Structure Calculations:
From Density Functional to Quantum Monte Carlo

Abstract: In the first part, a light overview of the electronic structure methods used in numerical molecular electronic structure calculations will be given. Namely,

- self-consistent field (SCF) known as Hartree-Fock (HF)
- density functional theory (DFT)
- configuration interaction (CI)
- multi-configurational SCF (MC-SCF)
- variational Monte Carlo (VMC)
- diffusion Monte Carlo (DMC)

will be introduced. The methods are ordered according to amount of electronic correlation they allow to recover in practice. Strategy to approach exact solutions of non-relativistic Schorödinger equation in Born-Oppenheimer approximation will be discussed.
In the second part, published results obtained by applying the introduced methods will be presented. Four topics will be covered (methods used are indicated):

- Mechanochemistry of thiolated copper clusters and surfaces (DFT)
- Magnetism in thiolated-gold cluster junctions (DFT)
- Spin states of vanadium-benzene (DFT, VMC, DMC)
- Excited states of of azobenzene (DFT, MC-SCF, VMC, DMC)

These topics may be divided according to various aspects to i) nature of systems of interest, organo-metallic (thiolated copper and gold clusters, vanadium-benzene) and organic (azobenzene); ii) methods used - mean-field (HF, DFT) and correlated (MC-SCF, VMC, DMC); iii) ground-state vs. excited states. All aspects will be briefly covered. Where possible, the results will be compared to experiment.