

SEMINARIUM RENTGENOWSKIE

Dnia 15.04.2014r. o godz. 10.30, w Sali D Instytutu Fizyki PAN, odbędzie się seminarium rtg., na którym **dr Paweł Rejmak** z Instytutu Fizyki PAN, wygłosi referat na temat:

"Hartree-Fock Method and Boldly Beyond"

Abstract:

The second talk of the introductory course to molecular modeling methods will focus on methods explicitly treating electronic structure. Schrödinger equation cannot be solved analytically for systems molecules, thus number of approximated methods have been introduced.

The first part of the talk will present the Hartree-Fock method, which employs wavefunction approximated as a determinant built of one electron functions (spinorbitals). Then the importance of Coulomb correlation, missed in Hartree-Fock approach, will be outlined and correlated methods of quantum chemistry will be briefly discussed.

dr hab. Sławomir Kret