

# SEMINARIUM RENTGENOWSKIE

Dnia 25.03.2014r. 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:

## "Exploration of Potential Energy Surface"

Abstract:

This is the first of intended series of talks giving introduction to molecular modeling in chemistry and physics.

This talk focuses on the concept of potential energy surface (PES) and the ways of finding for stationary points of this (hyper)surface. The scientific background behind PES, including Born-Oppenheimer approximation, will be explained, followed by short overview of computational techniques of minimization of energy. In the second part of the talk, the approximated way of computation of potential energy of molecules and solids, the molecular mechanics, will be covered.

Dr hab. Sławomir Kret