

SEMINARIUM RENTGENOWSKIE

Dnia 13.05.2014r. 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:

"Crash Course in The Density Functional Theory"

Abstract:

In the last talk of introduction to molecular modeling (too) short presentation of the density functional theory (DFT) will be given.

After quick overview of DFT prehistory and establishing formal background, given by Hohenberg-Kohn theorems, the most popular recipe for performing DFT calculations, Kohn-Sham method, will be discussed somewhat more in depth. The concept of exchange-correlation (xc) functional will be introduced, the ways of approximation of xc functionals and their performance are to be discussed.

Eventually, the reasons of DFT popularity will be revealed along with the explanation of several common DFT misunderstandings and superstitions.

dr hab. Sławomir Kret