SEMINARIUM RENTGENOWSKIE

Dnia 23.09.2014r. o godz. 10.30, w Sali D Instytutu Fizyki PAN, odbędzie się seminarium rtg. na którym **dr Yevgen Melikhov** z Instytutu Fizyki PAN, wygłosi referat na temat:

"Practical aspects of DFT calculations for solid state"

Short Abstract:

Density functional theory is a powerful *ab-initio* computational method used in physics and chemistry to investigate the electronic structure of many-body systems including solid state matter. Instead of solving Schrödinger equation to find wave functions directly, the method re-formulates the problem entirely so that minimization of a functional for the energy expressed in electron density is performed. At present, more than 70 computer programs distributed under Academic, Commercial or General Public Licenses are more-or-less actively used by the scientific community. After quick introduction to DFT method and explanation of the differences between various DFT programs, this talk will present the initial steps and practical aspects of usage of *mainly* Quantum Espresso, a software distributed under General Public License. In addition, this talk will cover some brief examples of DFT applications in solid state physics.

Dr hab. Sławomir Kret