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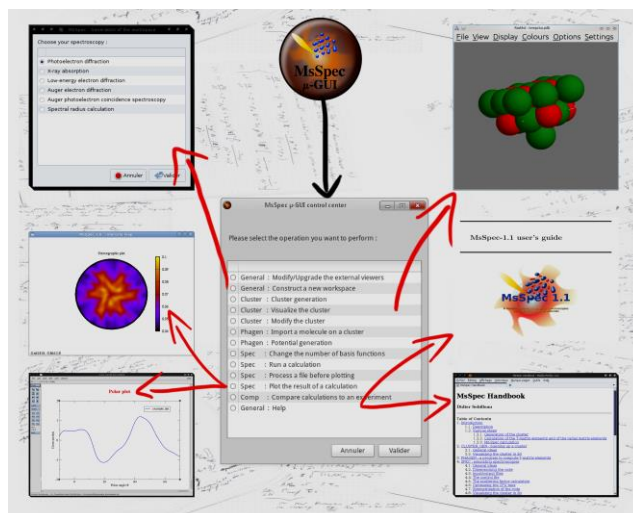
Photoelectron Diffraction Modeling within the MsSpec Package

by

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In this talk, I will present the MsSpec computer package, with a special focus on photoelectron diffraction. MsSpec is based on multiple scattering theory and can model at present five different spectroscopies. I will discuss the different algorithms underlying the package and give some examples of applications (photoelectron diffraction and Auger-photoelectron coincidence spectroscopy mainly). I will also describe some of the new features on which we are currently working and that will be incorporated into the next version of MsSpec, such as new spectroscopies, interface with ab initio codes, a new experiment-calculation comparison tool, Python embedding within the ASE (Atomic Simulation Environment) framework and a new GUI.



Date: 16 November 2017

Time: 10:00

Venue: Building G Vědeckotechnický park, TG 206, Teslova 9a, Pilsen

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