Seminar series: 27ᵗʰ, 28ᵗʰ and 29ᵗʰ March 2018, 10:00–11:30h
CFEL – Building 99, seminar room I and II (ground floor)

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Quantum mechanical calculations in angle-resolved photoelectron-ion coincidence spectroscopy

27.03.2018
Using the quantum mechanical programs to calculate molecule properties (GAUSSIAN, HyperChem, GAMESS ...)

Will be discussed the possibilities of computational chemistry and, especially, the quantum mechanical calculations of the molecule properties for the molecules in a gas phase. The main features and approximations used in quantum mechanical programs will be analyzed. For the GAUSSIAN and GAMESS programs it will be shown how to create the input file and display the calculated results.
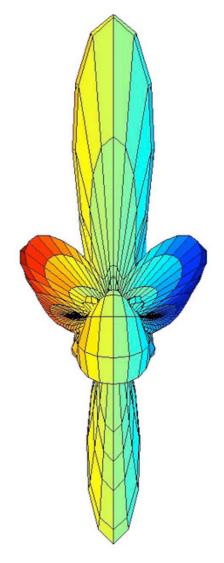
28.03.2018
Calculations of three dimensional photoelectron angular distributions with the MSXalpha program.

The Multi-Scattering Xalpha program significantly differs from the mainly used quantum mechanical programs (GAUSSIAN, GAMESS …). It gives the opportunity to calculate the three-dimensional photoelectron angular distributions, which can be experimentally measured in the photoelectron-ion coincidence experiments. The possibilities and the problems of the photoelectron-ion coincidence measurement will be reviewed and analyzed.

29.03.2018
Analysis of coincidence experimental data on the basis of GAUSSIAN and MSXalpha calculations.

The results of the Multi-Scattering Xalpha calculations for two conformers of 3-Hydroxychlorobenzene with different direction of O-H group relative to the main (C6H4Cl) part of molecule will be discussed. The dependence of the photoelectron angular distribution on the light polarization and the photoelectron energy will be analyzed. The possibility to take into account in the calculations the partial orientation of the molecule and the acceptance angle of the apparatus will be discussed.

Host: Jochen Küpper/ CFEL Molecular Physics Seminar