WWTF Project MA04-045

Ultrafast spectroscopy and time-dependent density functional theory

Abstract

Important future aspects of nanotechnology will be based on ultrafast properties of nano-scaled matter, e.g. magnetic switching. The goal of this project is to develop a fully relativistic ab-initio scheme within the time-dependent (current) density functional theory, that describes ultrafast phenomena occurring on a time scale of femtoseconds (10-15 s) in magnetic nano-systems characterized by a length scale of less than 10 - 20 nanometers (1 nm=10-9 m), like ultrafast demagnetization processes seen in pump-probe experiments. The involved re-search groups have both expertise in analysis and numerics for models for matter interact-ing with fields, in particular the time-dependent Dirac-Maxwell equations (mathematicians) and in calculating the magneto-optical properties of layered systems etc. (physicists). The project will be in close collaboration with one of the "founding fathers" of Density Functional Theory, Vienna born Walter Kohn.

Keywords:
ultrafast spectroscopie, nano solid state physics, time dependentdensity functional theory, partial differential equations in relativistic quantummechanics

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Funding volume: EUR 500,000

Further links about the involved persons and regarding the project you can find at
https://archiv.wwtf.at/programmes/mathematics/MA04-045