unicat
Unifying Concepts in Catalysis

UniCat Colloquium

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Quantum chemical calculations of magnetic resonance parameters

Magnetic resonance techniques are able to gain much insight regarding structure and bonding of molecules, molecular aggregates, and extended systems. In quantum chemistry, suitably chosen derivatives of the energy or the quasi-energy, e.g. with respect to electric and magnetic field amplitudes, nuclear spin magnetic moments and quadrupole moments, geometrical distortions, etc., give access to practically all spectroscopic and optical properties that are of interest in chemistry and related disciplines, including magnetic resonance parameters.
We give a brief overview of the computational approach and discuss selected applications for magnetic resonance parameters, with emphasis on metal complexes. The spectroscopic parameters of interest are NMR shifts and J-coupling, electric field gradients (quadrupolar interactions), electron paramagnetic resonance, chemical shifts of molecules with unpaired electrons, and nuclear spin relaxation rates.

Wednesday, May 13, 2015 at 5:15 PM
TU Berlin, Institute of Chemistry
Straße des 17. Juni 115, 10623 Berlin

Building C, Lecture Hall **C 264**

Prof. Kaupp (TUB)
Organizer

Coffee and cake will be served 30 minutes before the lecture. Guests are cordially invited to attend!
Prof. Dr. Matthias Driess - Chair of the Cluster of Excellence UniCat - www.unicat.tu-berlin.de