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Computational EPR Spectroscopy of Randomly Oriented Materials

APRIL, 24
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Seminar room **S2.02**
CEITEC BUT, Purkynova 123

Randomly oriented materials in form of powders, glasses or frozen solutions give rise to EPR spectra that usually are not easily amenable to direct quantitative analysis. In addition low symmetry environments often encountered in disordered heterogeneous systems can further complicate the spectra. Under such circumstances advanced computer analysis of the EPR spectra is the only method suitable for accurate extraction of the spin Hamiltonian parameters, allowing for their subsequent in-depth molecular interpretation. Computational EPR spectroscopy provides a combination of a hybrid genetic algorithm for robust and efficient simulation of complex experimental EPR spectra with density functional theory (DFT) calculations of magnetic parameters (g and A tensors or zero-field splitting). This approach can be used for guiding interpretation of the EPR data of large molecular and reticular paramagnetic systems characterized by complex structure, profound speciation, and low symmetry features. Appropriate level of theory of the relativity treatment along with careful selection of the exchange-correlation functional are indispensable for obtaining sensible results. The trustful experimental EPR parameters may guide the choice of proper calculation scheme to provide a quantitative connection between the molecular structure of investigated paramagnets and their spectroscopic fingerprints.
In this paper various aspects of computational EPR spectroscopy will be discussed and illustrated using examples coming from our laboratory.