

ZERNIKE INSTITUTE COLLOQUIUM

Thursday, April 1st, 2010

16:00h, Lecture Hall: 5111.0080

Coffee and cakes from 15:30h

Spin dependent effects in chemistry



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Open-shell transition metal ions display a number of distinct features in molecular electronic and magnetic spectra. While these can be probed by a large and powerful array of experimental methods, the interpretation of the experimental results is not always straightforward. Over the past years we have been involved in intense efforts to calculate these spectroscopic properties using wavefunction based methods as well as density functional linear response theory.

There have been numerous applications of the methods that have been developed in the framework of the ORCA program. In the lecture the present state-of-the art in the field will be present.

