CARL VON OSSIETZKY universität OLDENBURG
FAKULTÄT V
MATHEMATIK UND NATURWISSENSCHAFTEN

GDCh- und Chemisches Kolloquium

Der GDCh-Ortsverband Oldenburg und das Institut für Reine und Angewandte Chemie der Carl von Ossietzky Universität Oldenburg laden zu einem Vortrag

von Prof. Dr. Ria Broer
Zernike Institute for Advanced Materials
University of Groningen

zum Thema **The State of Transition Metals in Ionic Transition Metal Compounds**

herzlich ein.

Termin: **Donnerstag, den 23.10.2008 17 Uhr c.t.**
Großer Hörsaal der Naturwissenschaften, W3-1-161,
Carl-von-Ossietzky-Straße 9-11

Einladender Prof. Dr. Thorsten Klüner

Some transition metal compounds show technologically interesting properties like colossal magnetic resistance, ferroelectricity or temperature dependent magnetism. These properties are very sensitive to external stimuli like pressure. They are also believed to be connected to local distortions that are often present. In some cases different electronic states seem to co-exist, for example in rare earth manganites with a composition close to the metal-insulator transition. It is a challenge to study and analyze the competing mechanisms that determine these intriguing properties. Our approach will be illustrated with two examples. The first aims at designing photo-tunable magnetic materials. In this project we determine the mechanisms involved in the optical control of the magnetic properties of Prussian blue derivatives. The second project is aimed at tuning the properties of perovskite type oxides like CaFeO3, YNiO3 and LaMnO3. An important issue here is why seemingly similar materials show different distortions, such as charge disproportionation versus Jahn-Teller distortion and orbital ordering. A novel scheme to express CASSCF/CASPT2 wave functions in terms of optimized atomic orbitals is used to analyse the wave functions in Valence Bond terms. This turns out to be a practical tool to predict, for example, the type of distortions mentioned above.

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Der Vorsitzende
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