# The Intriguing Properties of Transition Metal Oxides.

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Many transition metal oxides show intriguing and technological useful properties like colossal magnetic resistance, ferroelectricity, multiferroicity, or superconductivity. These properties are believed to be critically dependent on details of the electron distributions around the transition metal ions and very sensitive to the local distortions that are often present, such as charge disproportionation, orbital ordering and Jahn-Teller distortion. Accurate theoretical studies of these properties require state-of-the-art quantum chemical calculations. Most of these studies are done using embedded clusters, but for some properties the cluster model is not adequate.

We developed a new method to treat crystalline materials including not only the effects of electron correlation but also the effects of delocalization over the crystal[1]. This *ab initio* many-electron periodic description uses a CASSCF treatment of large embedded cluster as a first step.

This new method is used to discuss the double exchange in the manganites $La_{1-x}Ca_xMnO_3$. We analyse the mechanisms that drive local geometry distortions in the perovskite type oxides $CaFeO_3$, $LaMnO_3$ and $YNiO_3$, using CASSCF/CASPT2 results for embedded clusters[2]. . Finally we discuss the electronic and magnetic properties of the high-temperature multiferroic CuO.

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Double exchange parameters in manganites, Int. J. Quant. Chem. 106 (2006) 2444-2457
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3. M. Pradipto, A. Nugroho and R. Broer, in preparation.