

# 21 世紀 COE セミナー

日時 : 2007 年 9 月 3 日 (月) 10 : 30 ~

場所 : 大阪大学大学院理学研究科 H 棟 6 階中セミナー室 (H601)

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題目 : Magnetic properties of free and supported transition metal clusters by magnetic circular dichroism in X-ray absorption

概要 : We present results of theoretical investigations on the electronic and magnetic properties of free and deposited transition metal clusters. A brief introduction to the applied techniques is given. These include, in particular, the Green's function method used for the electronic structure calculations within the framework of spin density functional theory (SDFT). As the approach is formulated in a fully relativistic way it gives access to all properties induced by spin-orbit coupling. This includes, in particular, a rigorous description for the magnetic circular dichroism in X-ray absorption that proved during the last years to be an outstanding tool to probe the magnetic properties of magnetic clusters. Concerning free clusters results for pure Fe and FePt compound clusters will be presented. The emphasis, however, will be put on deposited clusters as for example Co-clusters on a Pt(111) or Au(111) substrate. Beside clusters of magnetic atoms systems containing non-magnetic atoms are dealt with as well. These show induced magnetism if a magnetic atom is present as well but also spontaneous magnetism without a magnetic atom present. Another central issue will be the magnetic anisotropy induced by spin-orbit coupling and necessary to ensure stability against thermal fluctuations. Accordingly, all electronic and spectroscopic investigations are complemented by Monte Carlo simulations on finite temperature properties that are based on coupling constants calculated in an ab-initio way.

(担当 : 赤井研)