

## 21COE 物質階層融合科学セミナー 物性コロキウム

日時：12月7日(火) 16:30 - 18:00  
場所：理学部 総合研究棟 745号室(大学院講義室 )  
講師：Daniel Khomskii (Universitaet zu Koeln,  
Germany)  
題目：SITE- VS BOND-CENTERED ORDERING, PEIERLS  
STATE AND FERROELECTRICITY IN OXIDES

Abstract: In studying superstructures in transition metal oxides such as charge or orbital ordering, one usually considers site-centered superstructures. Such are for instance the standard checkerboard charge ordering in  $\text{La}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$ , or Verwey charge ordering in magnetite. However there exist another possibility: bond-centered superstructures, such as e.g. the Peierls state in low-dimensional systems. In this talk I will consider the possibility of competition or coexistence of site-centered and bond-centered structures on a few examples. One is the charge ordering in less-than-half-doped manganites. We have recently shown [1] that in this case indeed a bond-centered ordering may exist, and, moreover, bond-centered ordering may coexist with site-centered one, in which case the resulting state would be ferroelectric. This as a rare case of ferroelectricity in magnetic material - the so called multiferroic behaviour.

The second topic is an orbitally-driven Peierls state [2]. I will show that in spinels and in some other frustrated systems a site-centered orbital ordering (ODW-Orbital Density Wave) may lead to the formation of bond-centered singlet Peierls-like states. This picture gives a simple explanation of extremely strange superstructures observed recently in  $\text{MgTi}_2\text{O}_4$  [3] and  $\text{CuIr}_2\text{S}_4$  [4], and may be relevant for several other materials, such as  $\text{NaTiO}_2$ ,  $\text{La}_4\text{Ru}_2\text{O}_{10}$  [5] and some others. I will also give a general discussion in which cases bond-centered structures may be favourable.

#### [References]

- [1] D.Efremov, J.van den Brink and D.Khomskii, Nature Materials, in press
- [2] D.Khomskii and T.Mizokawa, cond-mat/0407458
- [3] M.Schmidt et al., Phys.Rev.Lett. 92, 056402 (2004)
- [4] P.G.Radaelli et al., Nature 416, 155 (2002)

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16:15 よりコーヒー、紅茶、お菓子を用意します。カップを持ってお集まり下さい。

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