21 世紀 COE
「京都大学化学連携研究教育拠点」
化学研究所・固体化学セミナー

講師：**Prof. Daniel I. Khomskii**
(Universitaet zu Koeln, Germany)

演題：**Orbitally-driven superstructures and spin gaps in spinels and other oxides**

日時：平成 18 年　8 月 14 日（月）14：00～
場所：化学研究所　新４Ｆセミナー室

Orbital degrees of freedom often lead to specific types of orbital and spin ordering. Complicated and interesting superstructures are observed in particular in B-sublattice of spinels. This is connected with the geometric frustration of this lattice and with the interconnection of edge-sharing MO_6 octahedra, which is especially important for transition metals with partially-filled t_{2g} levels. In some such systems ($MgTi_2O4$, $CuIr_2S_4$, AlV_2O_4) there appears strange superstructures with the formation of spin gap states. In other cases (ZnV_2O_4) structural transitions, apparently connected with orbital ordering, are followed by long-range magnetic ordering. Last but not least, the famous Verwey transition in magnetite Fe_3O_4 leads to a very complicated structural pattern, accompanied by the appearance of ferroelectricity. In this talk I will discuss all these examples, paying main attention to an interplay of charge, spin and orbital degrees of freedom. In particular, for $MgTi_2O_4$, and $CuIr_2S_4$ we proposed the picture of orbitally-driven Peierls state [1], which can be also relevant for several other materials, such as $NaTiO_2$, $La_4Ru_2O_{10}$ [2] and some others. Orbital ordering can also give rise to a spontaneous formation of Haldane chains in a three-dimensional systems like pyrochlore $Tl_2Ru_2O_7$ [4]. Finally, I propose the model of charge and orbital ordering in magnetite [4], which uses the idea of an interplay of site- and bond-centered ordering [5] and which seems to explain both the structural data and the presence of ferroelectricity in Fe_3O_4 below Verwey transition.

[1] D.I.Khomskii and T.Mizokawa, Phys.Rev.Lett. **94**, 156402 (2005);
[2] Hua Wu et al., Phys.Rev.Lett. 96, 256402 (2006)
[3] Seongsu Lee et al., Nature Mater. 5, 471 (2006)
[4] D.I.Khomskii, unpublished;
[5] D.V.Efremov, J.van den Brink and D.I.Khomskii, Nature Mater. **3**, 853 (2004)

世話人：無機先端機能化学　高野幹夫（内 3120）