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Orbital Superstructures in Spinel

DANIEL KHOMSKII, II.Physikalisches Institut, Universitaet zu Koeln

Orbital degrees of freedom often lead to specific types of orbital and spin ordering. Complicated and interesting superstructures are observed 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_2O_4 , 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]. Similar phenomenon can also explain situation in ZnV_2O_4 [2], although the corresponding superstructure has not yet been observed experimentally. Finally, I propose the model of charge and orbital ordering in magnetite [3], which uses the idea of an interplay of site- and bond-centered ordering [4] 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[2] Hua Wu, T.Mizokawa and D.I.Khomskii, unpublished;

[3] D.I.Khomskii, unpublished;

[4] D.V.Efremov, J.van den Brink and D.I.Khomskii, Nature Mater. **3**, 853 (2004)