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Orbital-selective singlet dimer formation and suppression of double exchange in 4d and 5d systems[1] SERGEY STRELTSOV, Institute of Metal Physics, GANG CAO, University of Kentucky, DANIEL KHOMSKII, University of Cologne — One of the main mechanisms of ferromagnetic ordering in conducting materials is the double exchange (DE). It is usually supposed in DE model that the Hunds coupling J_H is much larger than electron hopping t; in this case one stabilizes the state with maximum spin per pair of ions, which finally leads to ferromagnetism in bulk systems. We show that in the dimerized $4d/5d$ transition metal oxides for which J_H is reduced and t is in contrast enhanced, another situation is possible, when formation of the spin-singlets on delocalized orbitals is more favorable. This leads to suppression of the DE and to a strong decrease of the total spin. The model calculations using the dynamical mean-field theory show that this effect survives even in the extended systems, not only for dimers. Such a situation is realized, e.g., in $Y_5Mo_2O_{12}$, CrO_2 under pressure and in many other $4d/5d$ based materials. Another mechanism, which may suppress DE and which is also typical for $4d/5d$ compounds is the spin-orbit coupling (SOC). We show on the example of $Ba_5AlIr_2O_{11}$, that in this system it is the combination of molecular-orbital formation and SOC that strongly decreases magnetic moment on Ir.

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