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Modelling of phase transitions in the $R\mathrm{VO}_3$ perovskites

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Spin-orbital superexchange models provide a theoretical framework for describing magnetic and optical properties of Mott insulators with orbital degrees of freedom [1]. The spin-orbital superexchange model for $(xy)^1(yz/zx)^1$ configuration at each V^{3+} ion in $R\mathrm{VO}_3$ perovskites captures $\{yz, zx\}$ orbital fluctuations along the c axis [2]. The model that describes both orbital transition at $T_{\rm OO}$ and magnetic transition at T_{N1} to the C-type antiferromagnetic order has to include as well [3]: the crystal field, intersite orbital interactions, and the orbital-lattice coupling which all vary with ionic radius r_R. The decreasing r_R is accompanied by increasing GdFeO_3-like alternating rotations of the VO_6 octahedra by angles ϑ and φ, see inset in Fig. 1(a). This leads to the orthorhombic lattice distortion $u = (b-a)/a$, where a and b are the lattice parameters of the $Pbnm$ structure. The orthorhombic distortion u acts as a transverse field $gu\tau_i^x$ (τ_i^x is the orbital operator at site i, $g_{\rm eff} \equiv gu$), which acts as a transverse field on the orbitals and polarizes them, and therefore competes with orbital correlations induced by superexchange J [$J \simeq 200$ K in Fig. 1(a)]. While singlet orbital fluctuations are reduced at small values of r_R, the value of the Néel temperature T_{N1} is lowered in agreement with experiment, Fig. 1(a). Simultaneously, the nonmonotonic dependence of $T_{\rm OO}$ on r_R can be explained by a rapid increase of the orbital polarization $\langle\tau^x\rangle$ (or $g_{\rm eff}$), in agreement with the surprisingly large experimental increase of lattice distortions u_0 and u_1 from La to Y by one order of magnitude, see Fig. 1(b).

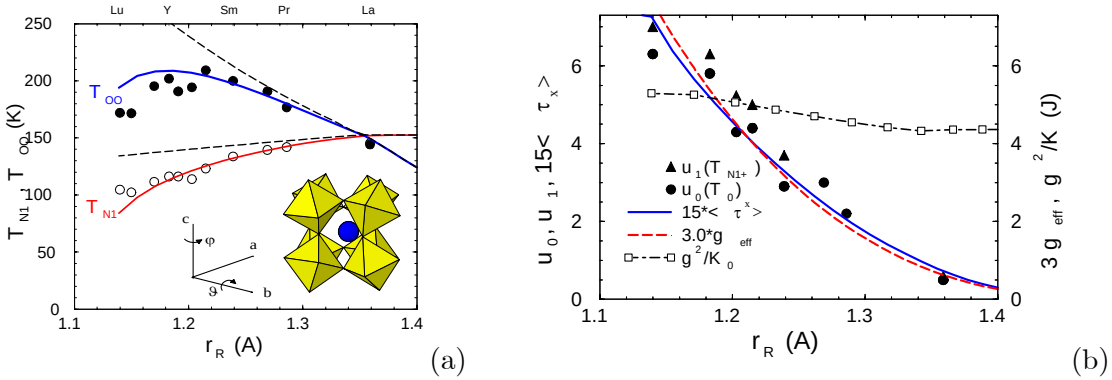

Figure 1: (a) The orbital transition $T_{\rm OO}$ and Néel temperature T_{N1} (solid lines) for varying ionic size r_R in $R\mathrm{VO}_3$ perovskites, as obtained from the theory [3], and from experiment (circles); dashed lines for $g_{\rm eff} = 0$. The inset shows the GdFeO_3-type distortion, with the rotation angles ϑ and φ. (b) Experimental distortion (in percent) at $T_0 = 0$ (u_0, circles) and above T_{N1} (u_1, triangles), compared with the orbital polarization $\langle\tau^x\rangle_{T=0}$ and with $g_{\rm eff}$. Squares show the upper bound for g^2/K predicted by the theory (at $u_0 = 0$).

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