Prediction of a strongly ferromagnetic layered insulator Sr_2NiRuO_4

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Abstract

A magnetic insulator is often antiferromagnetic, and a layered one normally has a low ordering temperature. Here we predict a surprising strong ferromagnetism (FM) in the layered insulator Sr_2NiRuO_4, using density functional calculations and spin-lattice Monte Carlo simulations. Our results show that Sr_2NiRuO_4 is in the S=1/2 Ni^+ and S=3/2 Ru^{3+} state. A strong intralayer FM coupling and a relatively weak interlayer FM one are demonstrated by density functional calculations, and using these exchange parameters, our Monte Carlo simulations give a high Tc of 240 K . All these results are in line with analyses of the crystal field level diagrams and the spin-orbital states of the square planar Ni^+ (S=1/2) and Ru^{3+} (S=3/2) ions. This work highlights a potential of unusual charge-spin-orbital states in producing novel magnetoelectric properties.

Results and Discussion

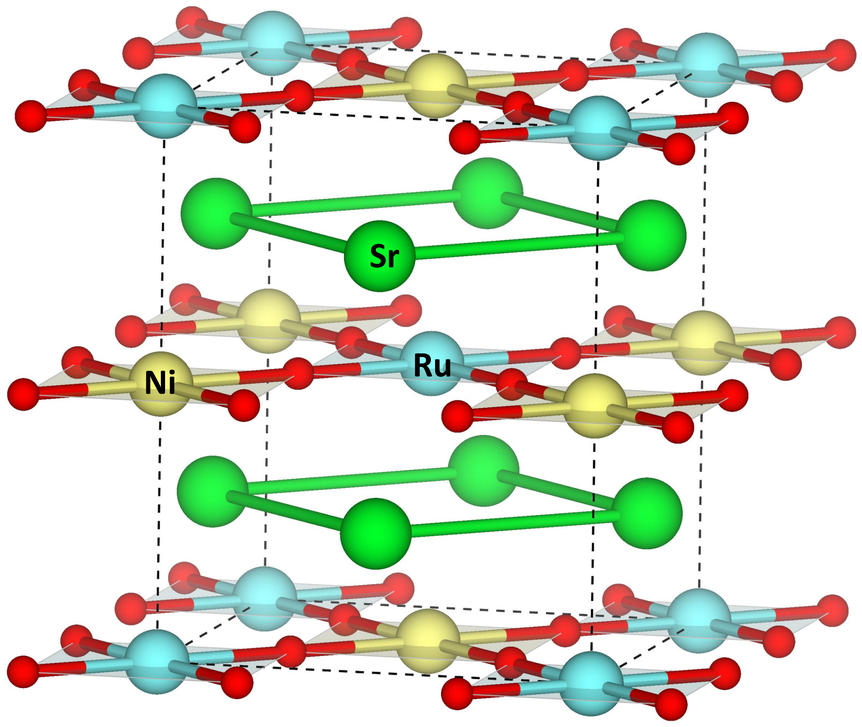

FIG. 1: (a) Crystal structure of the layered Sr_2NiRuO_4.

Sr_2NiRuO_4		ΔE	Tot	Ni	Ru
LSDA	FM	0	3.53	0.90	1.74
	A-AFM	18	0.00	0.82	1.65
	C-AFM	A-AFM			
LSDA+U	FM	0	4.00	1.13	2.09
	A-AFM	20	0.00	1.14	2.06
	C-AFM	162	0.00	0.74	1.95

Table. 1: Relative total energies ΔE (meV/f.u.), total and local spin moments (μ_B) of the FM, A-AFM, and C-AFM states calculated by LSDA and LSDA+U. J_{ab}= -27.0 meV and J_c= -6.67 meV are estimated.

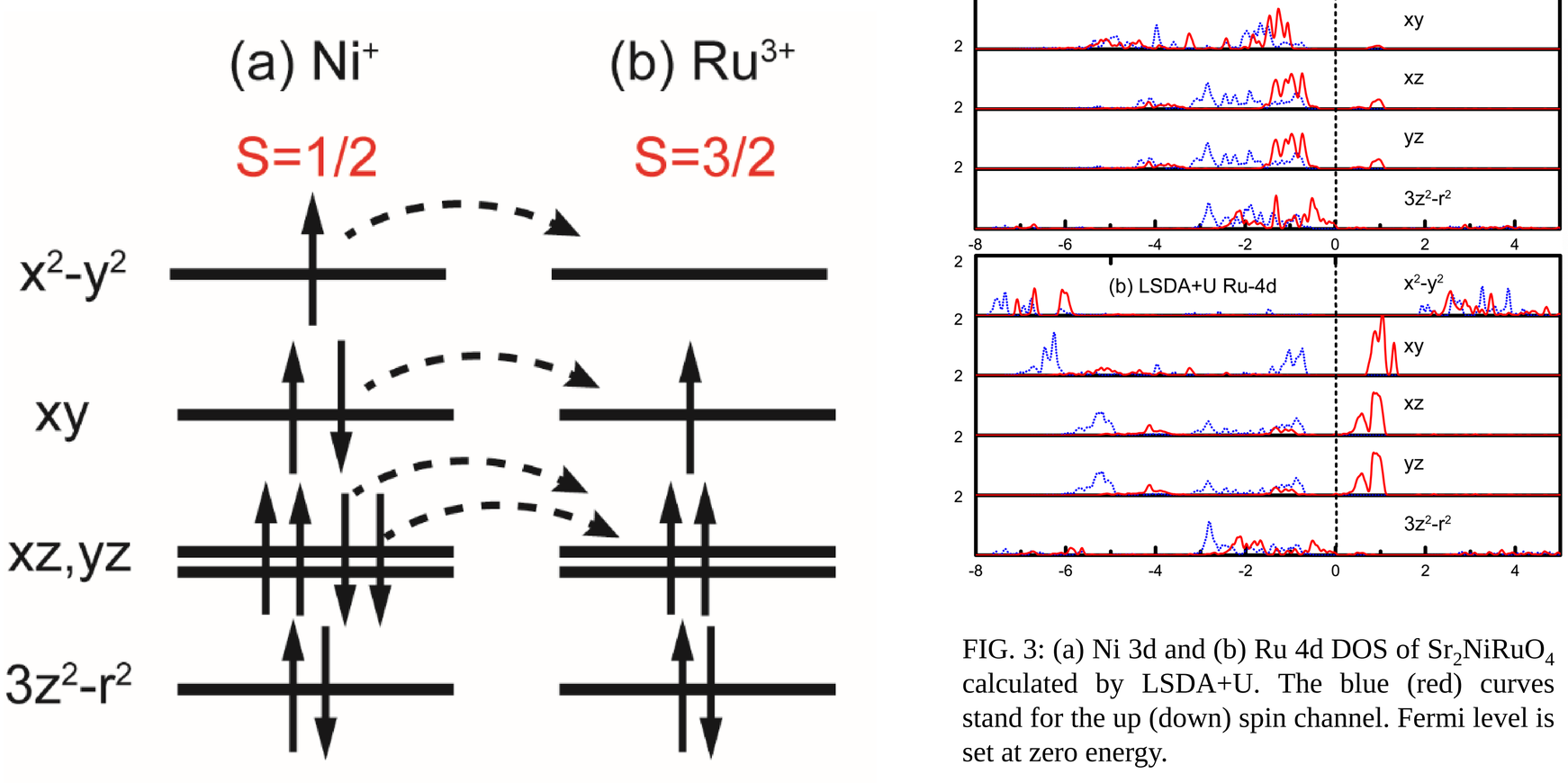

FIG. 2: Schematic crystal field level diagrams of (a) Ni^+ S=1/2, (b) Ru^{3+} S=3/2. Electron hoppings from Ni^+ to Ru^{3+} would yield a FM order.

FIG. 3: (a) Ni 3d and (b) Ru 4d DOS of Sr_2NiRuO_4 calculated by LSDA+U. The blue (red) curves stand for the up (down) spin channel. Fermi level is set at zero energy.

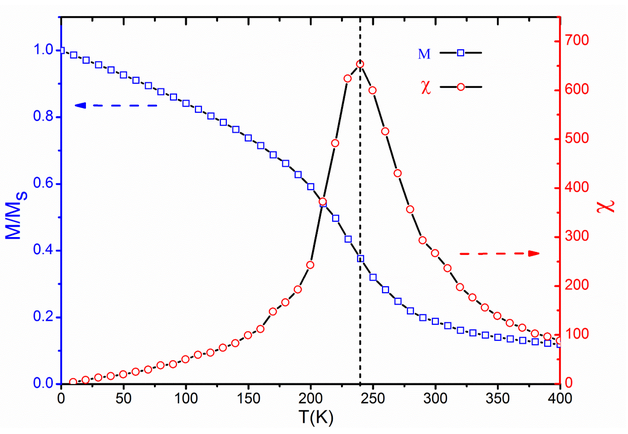

FIG. 4: Monte Carlo simulations of magnetization and magnetic susceptibility of Sr_2NiRuO_4 as a function of temperature. Tc is 240 K.

Conclusions:

(1) The layered insulator Sr_2NiRuO_4 has magnetic Ni^+ (S=1/2) and Ru^{3+} (S=3/2) ions.

(2) A strong intralayer FM coupling and a relatively weak interlayer FM one determine a high Tc via the special charge-spin-orbital states.