Supporting Information for

On the electronic structure required for the uniaxial magnetic properties of the magnetic metal $\text{SrCo}_6\text{O}_{11}$

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Figure S1. Occupations of the d-block energy levels of an isolated Co(3)O_5 TBP by a high-spin Co^{3+} (d^6) ion in (a), and a low-spin Co^{3+} (d^6) ion in (b).

Figure S2. DOS (per formula unit) representation of the electronic structure of $\text{SrCo}_6\text{O}_{11}$ from the GGA calculations with total moment of $4.64 \mu_B$ per FU, where the total DOS plot is represented by black line, the partial DOS plot for the Co atoms by blue line, and that for the O atoms by red line.

Figure S3. DOS (per formula unit) representation of the electronic structure of $\text{SrCo}_6\text{O}_{11}$ from GGA+U calculations with total moment of $4.01 \mu_{\text{B}}$ per FU, where the total DOS plot is represented by black line, the partial DOS plot for the Co atoms by blue line, and that for the O atoms by red line.

Figure S4. Partial DOS (per atom) plots of the d-orbital contributions of the Co(3) atom from the GGA calculations with total moment of $4.64 \mu_B$ per FU.

Figure S5. Partial DOS (per atom) plots of the d-orbital contributions of the Co(3) atom from the GGA+U calculations with total moment of $4.01 \mu_B$ per formula unit.

Table S1. Total moment of SrCo₆O₁₁ (per FU), net spin and orbital moments of the Co atoms (per atom) obtained from the GGA+SOC and GGA+U+SOC calculations for the ferromagnetic state of SrCo₆O₁₁ by one SCF iteration starting with the converged densities of the corresponding GGA and GGA+U calculations ^a

Method		Total moment	Co(1)	Co(2)	Co(3)	ΔE ^b
GGA+SOC	//c	3.99	0.37 (0.01)	0.19 (0.02)	1.70 (0.00)	0
	$\perp c$	3.98 ^c	0.37 (0.00)	0.19 (0.00)	1.70 (0.02)	-1700
	//c	5.98	0.50 (0.03)	0.39 (0.05)	2.36 (0.13)	0
	$\perp c$	5.97 ^c	0.50 (0.00)	0.39 (0.01)	2.36 (0.08)	-3500
GGA+U+SOC	//c	3.95	0.35 (0.01)	0.14 (0.01)	1.54 (-0.06)	0
	$\perp c$	3.80 ^c	0.33 (0.00)	0.14 (0.00)	1.51 (0.04)	-940

^a The orbital moments on Co(1), Co(2) and Co(3) atoms obtained from the calculations with SOC are given in parentheses.

^b $\Delta E = E_{\perp c} - E_{//c}$ (in meV), where $E_{\perp c}$ and $E_{//c}$ refer to the energies of the spin-orbit-coupled states with $\perp c$ and $//c$ spin orientations, respectively.

^c The SOC calculations with $\perp c$ spin orientation give rise to two slightly different Co(1) sites. The net spin and orbital moments listed are their average values.