The four Cu_2Sb-type compounds: Mn, Co and As, Sb

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Antiferromagnetic spintronics [1] needs thin layers...

Motivated by the utility of CuMnAs [2] in this field, we look at other materials of the same structure that could possibly be grown epitaxially. We begin with Mn_2Sb which is, in the ground state, ferrimagnetic. In bulk, this is a well known material. Interestingly, by alloying Sb with As, it transforms into an antiferromagnet [3] (which can, however, return to the ferrimagnetic state upon increasing temperature). Simple DFT yields the following energetics (in mRy/f.u.):

	ΔE	remark
ferri	0	
FM	15.4	unconverged
AFM1	12.6	...
AFM2		... the same

Magnetic moments (mmoms) depend only weakly on the type of magnetic order: Mn mmom at 2a Wyckoff position is smaller (about 2.9 μ_B) and the other (at 2c) is about 3.7 μ_B.

References

[1] RMP 90, 015005

[2] PRB 97, 125109

[3] Shirakawa and Ido, doi: 10.1143/JPSJ.40.666