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Noncollinear magnetism in antiferromagnetic manganese chalcogenides KOHJI NAKAMURA, TORU AKIYAMA, TOMONORI ITO, Mie University, A.J. FREEMAN*, Northwestern University — Metastable zincblende compounds of transition-metal pnictides and chalcogenides have recently become the subject of much attention due to their unique properties exhibiting combinations of magnetism and semiconductivity. Here we investigate magnetism in the antiferromagnetic (AFM) transition-metal chalcogenides, namely MnSe and MnTe, by using the FLAPW method.[1] Assuming a collinear magnetic structure, we demonstrate that the AFM structure consisting of alternating Mn (001) spin-up and spin-down planes is favored over the ferromagnetic state, since the majority-spin d-bands are completely filled and so achieve the half-filling state that leads to the superexchange interaction. However, with FLAPW calculations that now treat full noncollinear magnetism,[2] we find that the lowest energy state is a noncollinear AFM structure — the so-called AFM type III structure — which relaxes frustration in the AFM Mn moment alignment on the fcc sublattice, a result that agrees with neutron experiments.[3] *Supported by NSF MRSEC through the NU MRC.

[1]Wimmer, *et al.*, PRB 24, 864(1981)
[2]Nakamura, *et al.*, PRB 65, 12402 (2002); 67, 14420 (2003)
[3]Samarth, *et al.*, PRB 44, R4701 (1991)

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