Comment on "Magnetization Compensation Temperature and Frustration-Induced Topological Defects in Ferrimagnetic Antiperovskite Mn_4N"

Bayaraa *et al.*'s Letter [1] presents density functional theory calculations and Monte Carlo simulations for binary Mn_4N, based on a hypothetical tetragonal collinear magnetic structure. The authors claim a ferrimagnetic compensation point at 496 K, with hedgehoglike topological spin defects. However, their assumption contradicts extensive evidence that Mn_4N is a noncollinear cubic ferrimagnet with a triangular spin structure [Fig. 1(a)] and no magnetic compensation.

The authors consider two collinear structures (A and B) in their analysis, quoting a secondary source [2] that refers back to the 1962 neutron study [3]. Takei *et al.* [3] had deduced a collinear ferrimagnetic structure from their data (type A) with manganese moments of 3.85 μ_B on the 1a corner sites and −0.90 μ_B on the face-center 3c sites, which each have two nitrogen neighbors at the 1b body-center sites of the Pm-3m space group. No experimental evidence has been found for the type B collinear magnetic model favored by Bayaraa *et al.* [Fig. 1(b)] in the cited references [2] and [4]. Model B involves a small tetragonal distortion ($c/a \approx 0.99$) and very different magnetic moments for manganese on the Mn_{II} and Mn_{III} sites (1.16 μ_B and −3.01 μ_B), whose Mn-N distances differ by only 1%. In cubic symmetry the two sites are crystallographically equivalent and expected to have the same magnetic moment. Two, not three inequivalent Mn sites are seen in NMR [5], consistent with type A order. The inconsistency was clearly flagged in Ref. [2]. Nevertheless, Bayaraa *et al.* proceed to evaluate 45 exchange constants, four Dzyaloshinskii-Moriya exchange vectors, and six anisotropy constants based on a false hypothesis that leads them to predict compensation with "striking metastable topological states".

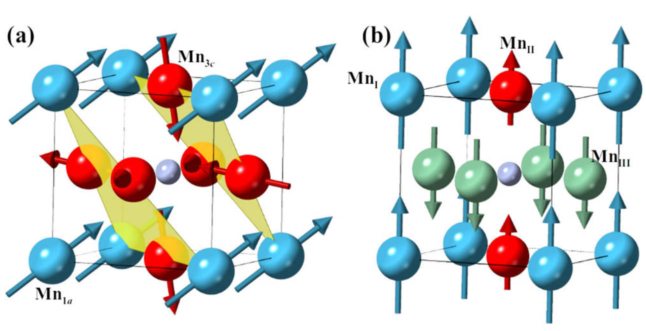

FIG. 1. Triangular spin structure of cubic Mn_4N (a) versus a hypothetical type "B" collinear tetragonal spin structure (b). The nitrogen atom is gray. Other colors distinguish Mn atoms with different magnetic moments.

A later study with polarized neutrons by Fruchart *et al.* [6], confirmed by DFT calculations [7], found that the magnetic structure is actually a noncollinear variant of type A. The 3c moments of Mn lie on a frustrated kagome lattice with components in the plane perpendicular to the $\langle 111 \rangle$ ferrimagnetic axis that are oriented at 120° to each other. Analogous cubic Mn_3M' compounds with $M' =$ Rh, Ir, or Pt are triangular antiferromagnets [8]. The absence of compensation in Mn_4N has been repeatedly confirmed over the past 60 years [6,7,9–12].

The likely topological character of the magnetism in these structures was pointed out by Bertaut in the 1970s [13], when ternary metallic perovskites $M_3M'Z$, $Z =$ N, C were intensively investigated. These results and many others compiled in a volume of Landolt-Börnstein [14] provide the basis of our current understanding of this interesting family of metallic magnets. Unfortunately, the calculations of Bayaraa *et al.* disregard what was already known about the structure and magnetism of Mn_4N.

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