

Erratum: Generation of Pure Spin Current with Insulating Antiferromagnetic Materials [Phys. Rev. Lett. 135, 146703 (2025)]

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In the original Letter, an incorrect result regarding the high-throughput screening was presented due to a bug in our code that misidentified the magnetic point groups of several materials. Specifically, materials possessing type-IV magnetic space groups (which include the antitranlation operation, a translation $\mathbf{t}$ combined with a spin reversal, written as $\{1'|\mathbf{t}\}$ in Seitz notation) were erroneously included. This operation forbids the piezospintronic effect. Excluding these compounds reduces the number of valid candidates from the original 85 to 56. After correcting this error, we have verified that the magnetic point groups of the candidate materials are now consistent with those listed in the MAGNDATA database [1–2].

The revised high-throughput screening workflow is shown in Fig. 1 (which replaces Fig. 3 in the original Letter). The total number of candidate materials is now 61 (comprising 56 of the original valid candidates plus 5 newly identified materials), as detailed in Table I (which replaces Table S2 in the original Supplemental Material). These candidates consist of 51 collinear and 10 noncollinear magnetic materials. Furthermore, symmetry analysis based on magnetic and spin point groups reveals that none of the candidate materials exhibit piezospintronic effects induced by spin-orbit coupling.

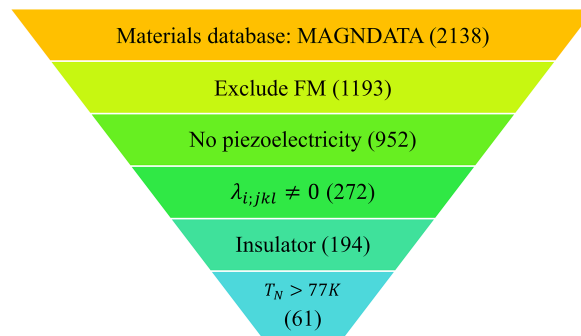


FIG. 1. The high-throughput screening workflow. The number of materials remaining at each stage of the process is indicated in parentheses.

TABLE I. Candidate materials for the piezospintronic effect identified through the high-throughput screening. The table includes the following columns: the number, the material label in MAGNDATA, the number of sites in the calculation cell, the reduced chemical composition, the Néel temperature recorded in MAGNDATA, and whether the magnetic structure is noncollinear.

No.	Label	Sites	Reduced composition	T_Neel	Noncollinear
1	0.464	5	Ba1 Mn2 P2	?	False
2	0.470	5	Ba1 Mn2 Sb2	443	False
3	0.92	5	Ca1 Mn2 Sb2	83	False
4	0.523	5	Ca1 Mn2 Sb2	85	False
5	0.482	5	Sr1 Mn2 As2	118	False
6	0.618	6	K1 Mn1 Bi1	<295	False
7	0.617	6	K1 Mn1 Sb1	<295	False
8	0.629	6	Na1 Mn1 As1	>293	False

(Table continued)

TABLE I. (*Continued*)

No.	Label	Sites	Reduced composition	T_Neel	Noncollinear
9	0.630	6	Na1 Mn1 As1	>293	False
10	0.634	6	Na1 Mn1 Bi1	>293	False
11	0.635	6	Na1 Mn1 Bi1	>293	False
12	0.626	6	Na1 Mn1 P1	>293	False
13	0.627	6	Na1 Mn1 P1	>293	False
14	0.628	6	Na1 Mn1 P1	>293	False
15	0.631	6	Na1 Mn1 Sb1	>293	False
16	0.632	6	Na1 Mn1 Sb1	>293	False
17	0.633	8	Fe1 K1 S2	250	False
18	0.636	8	Fe1 Rb1 S2	188	False
19	0.638	8	Fe1 Rb1 Se2	249	False
20	0.186	8	Ce1 Mn1 As1 O1	347	False
21	0.665	8	Ce1 Mn1 Sb1 O1	240	False
22	0.212	9	As2 Mn3 O2 Sr2	340	False
23	0.110	10	Cr2 O3	307.6	False
24	0.125	10	Ge1 Mn1 O3	120	False
25	0.163	10	Mn1 P1 S3	78	False
26	0.399	16	Fe1 H1 O2	340–440	False
27	0.76	18	Cr2 Te1 O6	93	False
28	0.143	18	Cr2 Te1 O6	?	False
29	0.959	18	Cr2 Te1 O6	105	False
30	0.142	18	Fe2 Te1 O6	219	False
31	0.960	18	Fe2 Te1 O6	218.5	False
32	0.401	19	Fe4 O11 Sr4	232	False
33	0.733	20	Ag1 O3 Ru1	342	False
34	0.208	23	Fe8 Se10 Ti5	100	False
35	0.209	23	Fe8 Se10 Ti5	500	False
36	0.969	28	Ca1 Fe2 O4	200	False
37	0.442	30	Fe4 Nb2 O9	90	False
38	0.443	30	Nb2 Fe4 O9	94	False
39	0.507	30	Mn4 Nb2 O9	125	False
40	0.477	30	Ta2 Mn4 O9	106.4	False
41	0.526	30	Ta2 Mn4 O9	110	False
42	0.692	34	Ba4 O10 Ru3	105	False
43	0.693	34	Ba4 O10 Ru3	108.0	False
44	0.801	36	Ti3 Fe2 S4	90	False
45	0.814	36	Fe2 W1 O6	235.7	False
46	0.1001	60	Mn2 Ni6 Te3 Pb1 O18	86	False
47	0.457	64	Cs1 Fe1 O2	350	False
48	0.459	64	K1 Fe1 O2	1001	False
49	0.460	64	K1 Fe1 O2	960	False
50	0.455	64	Rb1 Fe1 O2	737	False
51	0.386	72	Fe3 B1 O5	112	False
52	0.987	12	Ba1 Fe2 S2 O1	250	True
53	0.988	12	Ba1 Fe2 Se2 O1	240	True
54	0.762	12	Sr1 Fe2 S2 O1	216	True
55	0.924	24	Rb1 Ru1 O4	?	True
56	0.441	30	Nb2 Fe4 O9	97	True
57	0.809	36	Fe2 W1 O6	264	True
58	0.819	36	Mn1 Nb2 O6	?	True
59	0.806	88	Fe2 Se2 O7	105	True
60	0.807	88	Fe2 Se2 O7	105	True
61	0.808	88	Fe2 Se2 O7	105	True

We subsequently performed first-principles calculations on these new candidates. Our calculations show that the piezospintronic effects of KFeS_2 and SrMn_2As_2 are not large, and the band gaps of $\text{TlFe}_{1.6}\text{Se}_2$ and $\text{Sr}_4\text{Fe}_4\text{O}_{11}$ are very small. Consequently, the primary findings of the study remain unchanged.

We also wish to clarify that in the final step of the high-throughput screening, to ensure suitability for practical device applications, we excluded materials with a Néel temperature below 77 K as well as those containing rare-earth elements.

Finally, we correct several notations in Table I in the original Letter: the magnetic point groups $4/m'm'm$, $2'2'2'$ and $6/m'm'm$ should be corrected to $4'/m'm'm$, $2'2'2$ and $6/m'm'm'$, respectively.

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- [1] S. V. Gallego, J. M. Perez-Mato, L. Elcoro, E. S. Tasci, R. M. Hanson, M. I. Aroyo, and G. Madariaga, MAGNDATA: Towards a database of magnetic structures. II. The incommensurate case, *J. Appl. Crystallogr.* **49**, 1941 (2016).
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