

Can Public DFT Databases Guide Composition Selection for Metastable Magnets? A Validation of Energy-Above-Hull Screening Against Rapidly Solidified and Milled TbCu₇-Type Sm–Fe–M Alloys

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Public density-functional-theory (DFT) databases are increasingly used to screen compositions for permanent magnets. Yet it remains unclear how reliably their stability predictions apply to metastable phases produced by non-equilibrium processing. Here, we compare six public resources—Materials Project, AFLOW, JARVIS-DFT, NOMAD/Alexandria, OQMD, and GNoME—against published phase observations for melt-spun and mechanically milled Sm–Fe and Sm–Fe–M alloys (M = Co, Ti, V, Zr, Nb, Cu, Si, Ga, Al, Mo, Cr, Mn, or Hf). The database snapshot contains 628 entries; 30 of 38 curated literature observations can be scored across 11 alloy systems. Because none of the databases explicitly represents disordered TbCu₇, we construct a stability proxy from the lower convex envelope of available ordered CaCu₅, 2:17, 3:29, and ThMn₁₂ relatives, measured against each database’s own convex hull. We also estimate the ideal configurational-entropy contribution. Materials Project, OQMD, and Alexandria place no binary Sm–Fe compound on their respective hulls. They assign closely spaced energies to equilibrium Sm₂Fe₁₇ (19.4–22.9 meV/atom), metastable TbCu₇-type SmFe₉ (proxy: 15.6–19.3 meV/atom), and SmFe₁₂ (18.6–23.7 meV/atom), which is not obtained as a bulk ThMn₁₂ phase by the melt-spinning routes considered. Their maximum separation is only 4.4 meV/atom, and the proxy for metastable SmFe₉ is ranked below equilibrium Sm₂Fe₁₇. Consequently, their high hit rates at a 50 meV/atom threshold (20–24 hits, with at most one miss) do not establish an ability to distinguish phase-forming outcomes. JARVIS-DFT gives the expected ordering but places the SmFe₉ proxy at 89.4 meV/atom, missing 19 of 20 covered positive observations. AFLOW and GNoME provide no comparable matches, and the screened resources contain no explicit disordered TbCu₇, ω , or Sm₅Fe₁₇ entries. Interpolated Fe moments for SmFe₉ differ from a measured value extrapolated to 0 K (1.88–1.96 μ_B /Fe) by +16% for Alexandria and –22% for JARVIS-DFT. These results show that energy above hull, as currently exposed by the databases examined, is insufficient by itself to select metastable Sm–Fe–M phases. We recommend checking whether a database reproduces known equilibrium phases before applying formability thresholds and provide the underlying proxy table, validation matrix, and reproducible pipeline.

Keywords: permanent magnets; TbCu₇ structure; Sm–Fe–N; metastable phases; rapid solidification; mechanical alloying; energy above hull; high-throughput DFT; database validation

I. INTRODUCTION

Permanent magnets are essential to electric motors, wind generators, actuators, and sensors. Many high-performance applications rely on rare-earth elements [1]. In particular, Nd–Fe–B magnets, including high-coercivity grades containing Dy or Tb, create demand for elements with geographically concentrated supply chains [1,2]. This has renewed interest in alternative magnets that reduce dependence on these elements without sacrificing performance. Samarium–iron alloys are a promising and well-established family. Nitrogenation of Th₂Zn₁₇-type Sm₂Fe₁₇ produces Sm₂Fe₁₇N₃, which exhibits strong uniaxial anisotropy and a substantially higher Curie temperature than the parent alloy [2,3].

The hexagonal TbCu₇-type family offers another route to Fe-rich magnets. With compositions typically between SmFe₇ and SmFe₁₀, these alloys contain more Fe per Sm atom than Sm₂Fe₁₇, while their nitrides can exhibit high saturation polarization and magnetic anisotropy [2,4–7,50]. Their main limitation is metastability: TbCu₇ is not an equilibrium phase of the binary Sm–Fe system.

Instead, it is commonly obtained by rapid solidification or mechanical alloying followed by controlled annealing [4,8–11]. Katter et al. observed TbCu_7 in binary Sm–Fe ribbons only above a wheel speed of approximately 15 m/s; slower quenching or higher Sm content favored the equilibrium $\text{Th}_2\text{Zn}_{17}$ structure [4]. Additions such as Zr, Co, V, Nb, and Ga can broaden the processing window for TbCu_7 formation and improve magnetic properties. Room-temperature polarization exceeding 1.7 T has been reported for $(\text{Sm,Zr})(\text{Fe,Co})_{10}$ [5,6,12–16].

Structurally, TbCu_7 is the disordered parent of a whole family of rare-earth–transition-metal compounds. Starting from the CaCu_5 structure (space group $P6/mmm$), a fraction δ of the rare-earth sites is replaced at random by pairs (“dumbbells”) of transition-metal atoms aligned with the c axis, giving the general formula $\text{R}_{1-\delta}\text{T}_{5+2\delta}$. When the dumbbells order, the same substitution produces rhombohedral $\text{Th}_2\text{Zn}_{17}$ and hexagonal $\text{Th}_2\text{Ni}_{17}$ at $\delta = 1/3$, the monoclinic 3:29 structure at $\delta = 2/5$, and tetragonal ThMn_{12} at $\delta = 1/2$ [2]. The ThMn_{12} member SmFe_{12} has outstanding intrinsic properties but has been obtained in the binary system only as thin films; bulk ThMn_{12} alloys require a stabilizing element such as Ti, V, Mo or Si [17–21]. Rapid solidification at the SmFe_{12} composition gives an amorphous ribbon or a $\text{TbCu}_7 + \alpha\text{-Fe}$ mixture rather than the ThMn_{12} phase [22,23].

In parallel with this experimental history, open high-throughput density-functional-theory (DFT) databases have become a routine first step in choosing compositions. Materials Project (MP) [24], AFLOW [25], JARVIS-DFT [26], the NOMAD repository [27], which hosts the Alexandria calculations [28], the Open Quantum Materials Database (OQMD) [29,30] and Google DeepMind’s GNoME predictions [31] together contain millions of computed structures. Their central screening descriptor is the energy above the convex hull, E_{hull} , the energy by which a compound lies above the lowest-energy combination of competing phases at the same composition. Analyses of experimentally known compounds show that most synthesized metastable materials lie within a few tens of meV/atom of the hull [32,33], and windows of 25–100 meV/atom are therefore widely used to flag candidates as “synthesizable” [32–34].

Two issues complicate the application of conventional energy-above-hull screening to TbCu_7 magnets. First, TbCu_7 involves chemical disorder, whereas the available database entries generally describe ordered cells. Its energy therefore cannot be read directly from these resources. Second, reliable energetics for rare-earth intermetallics are challenging because of partially filled 4f states, the choice of reference energies, and differences among computational treatments [34]. These limitations raise a practical question: can database-derived stability metrics distinguish phases formed by rapid quenching from closely related phases that are not obtained by the same route?

This work provides that test for Sm–Fe and Sm–Fe–M alloys, with M drawn from thirteen common stabilizing and substituting elements (Co, Ti, V, Zr, Nb, Cu, Si, Ga, Al, Mo, Cr, Mn, Hf). Its contributions are:

1. a reproducible, hash-verified snapshot of all 628 Sm–Fe(–M) entries in six public DFT databases, retrieved through keyless public interfaces;
2. a curated table of 38 literature observations of phases formed by melt spinning or mechanical alloying, of which 30 are scorable in 11 alloy systems;
3. a database-consistent stability proxy for the disordered TbCu_7 phase, built from each database’s own ordered relatives and referenced to its own convex hull, with an explicit configurational-entropy correction;
4. a validation of each database on five criteria: structure coverage, hull fidelity for known equilibrium phases, hit rate against observed phases, discrimination between phases of different experimental fate, and computed Fe moments.

The archived dataset, stability proxies, validation matrix, and analysis scripts are publicly available [35].

Section II introduces the structural framework and the TbCu_7 stability proxy. Section III describes database retrieval, literature curation, and the validation criteria. Section IV presents the results, including coverage, hull fidelity, phase discrimination, and magnetic-moment comparisons. Section V discusses their implications for screening, and Section VI concludes.

II. STRUCTURAL AND THERMODYNAMIC FRAMEWORK

A. The TbCu₇ family and its ordered derivatives

TABLE I: Members of the TbCu₇ structure family considered here, with the dumbbell fraction δ [Eq. (2)] and the Fe fraction f [Eq. (3)] of the binary Sm–Fe compound.

Class	Example	Struct.	x	δ	f
1:5	SmFe ₅	CaCu ₅	5	0	0.833
2:17	Sm ₂ Fe ₁₇	Th ₂ Zn ₁₇ /Th ₂ Ni ₁₇	8.5	1/3	0.895
TbCu ₇	SmFe ₉	TbCu ₇ (disord.)	9	4/11	0.900
3:29	Sm ₃ Fe ₂₉	Nd ₃ (Fe,Ti) ₂₉	9.67	2/5	0.906
1:12	SmFe ₁₂	ThMn ₁₂	12	1/2	0.923

We describe every rare-earth–transition-metal compound in the family by the ratio

$$x = \frac{N_T}{N_R}, \quad (1)$$

where N_T and N_R are the numbers of atoms on transition-metal and rare-earth sites, respectively. For the TbCu₇ formula R_{1- δ} T_{5+2 δ} one has $x = (5+2\delta)/(1-\delta)$, which inverts to

$$\delta = \frac{x-5}{x+2}. \quad (2)$$

The Fe atomic fraction of a binary Sm–Fe compound is

$$f = \frac{x}{1+x}, \quad (3)$$

and one formula unit contains $6+\delta$ atoms. Table I lists the ordered derivatives used in this work. The observed TbCu₇ phase in binary melt-spun Sm–Fe lies close to SmFe₉ ($x = 9$, $\delta = 4/11$) [4], between the 2:17 ($x = 8.5$) and 3:29 ($x \approx 9.67$) compositions.

B. Formation energy, convex hull and energy above hull

For a compound c with N_i atoms of element i and total energy E_c , the formation energy per atom is

$$E_f(c) = \frac{E_c - \sum_i N_i \mu_i^0}{\sum_i N_i}, \quad (4)$$

where μ_i^0 is the reference energy per atom of element i in its standard state. In a binary system the convex hull $H(f)$ is the lower convex envelope of the points $\{f_c, E_f(c)\}$ together with the two elements at $E_f = 0$. The energy above hull is then

$$E_{\text{hull}}(c) = E_f(c) - H(f_c) \geq 0, \quad (5)$$

and compounds with $E_{\text{hull}} = 0$ are predicted stable at zero temperature. Any systematic error in μ_{Sm}^0 shifts E_f of every Sm–Fe compound by an amount proportional to its Sm fraction, $1-f$. This dependence is central to the interpretation in Sec. V.

C. A stability proxy for the disordered TbCu₇ phase

No database contains a disordered TbCu₇ cell. We therefore estimate its energy from each database's own ordered relatives. Let $\{f_k, E_{f,k}\}$ be the Sm–Fe entries of a database that belong to the TbCu₇ family (CaCu₅, 2:17, 3:29, ThMn₁₂ and other Fe-rich approximants with $5.3 < x < 12.3$), and let $E_{\text{env}}(f)$ be their lower convex envelope. The TbCu₇ stability proxy is

$$\Delta E_{\text{TbCu}_7}(x) = E_{\text{env}}(f) - H(f), \quad f = \frac{x}{1+x}, \quad (6)$$

that is, the energy above the database's own hull of the best ordered arrangement of Sm atoms and Fe dumbbells available to that database at the same composition. Because the envelope uses only ordered cells, Eq. (6) omits the enthalpy cost of disordering the dumbbells, and therefore does not directly predict the enthalpy of the disordered phase. Without explicit disordered configurations, this envelope cannot be established as a rigorous bound.

D. Configurational entropy

Random occupation of the 1a site by Sm atoms (fraction $1-\delta$) and Fe dumbbells (fraction δ) adds an ideal configurational entropy per atom

$$\frac{S_{\text{conf}}}{k_B} = \frac{-\delta \ln \delta + (1-\delta) \ln (1-\delta)}{6+\delta}, \quad (7)$$

which lowers the free energy of the disordered phase at the processing temperature T :

$$\Delta G_{\text{TbCu}_7}(x, T) = \Delta E_{\text{TbCu}_7}(x) - T S_{\text{conf}}(x). \quad (8)$$

At $x = 9$ ($\delta = 4/11$), Eq. (7) gives $S_{\text{conf}} = 0.103 k_B$ per atom, and at $T = 1273$ K, a representative temperature for the melt just before it is quenched, $T S_{\text{conf}} = 11.3$ meV/atom. Because the ideal-mixing term assumes no short-range order, $T S_{\text{conf}}$ is an upper bound on the entropic stabilization.

E. Converting measured polarization to an Fe moment

To compare measured magnetization with computed moments, the saturation polarization J_s of the TbCu_7 phase is converted to an average Fe moment,

$$m_{\text{Fe}} = \frac{J_s V}{\mu_0 \mu_B N_{\text{Fe}}}, \quad V = \frac{\sqrt{3}}{2} a^2 c, \quad (9)$$

where V is the volume of the hexagonal TbCu_7 cell, a and c are the measured lattice parameters, and $N_{\text{Fe}} = 5+2\delta$ is the number of Fe atoms per cell. The Sm contribution is neglected. The room-temperature value is scaled to 0 K with Kuz'min's expression for the spontaneous magnetization [36],

$$\frac{m(\tau)}{m(0)} = [1 - s \tau^{3/2} - (1-s) \tau^{5/2}]^{1/3}, \quad \tau = \frac{T}{T_C}, \quad (10)$$

with the shape parameter s varied over 0.3–0.7 to bracket the unknown value. Computed moments at $x = 9$ are interpolated linearly in f between the two ordered parents that bracket the energy envelope,

$$m(f) = (1-w) m_1 + w m_2, \quad w = \frac{f - f_1}{f_2 - f_1}. \quad (11)$$

III. DATA AND METHODS

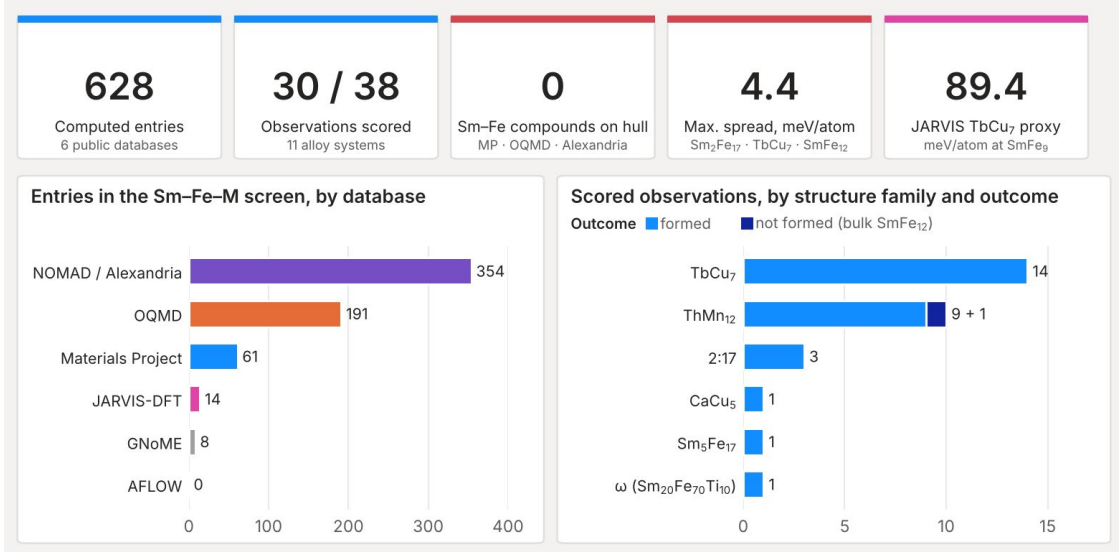


FIG. 1: Overview of the screen. Top: headline indicators. Bottom left: number of Sm-Fe(-M) entries retrieved from each database. Bottom right: the 30 scored observations by tested structure family and outcome. Data: archived snapshot of 13 October 2026 [35].

TABLE II: Coverage of the Sm-Fe-M space in six public DFT databases (snapshot of 13 October 2026). “ TbCu_7 family” counts CaCu_5 , 2:17, 3:29, ThMn_{12} and other Fe-rich approximants with $5.3 < x < 12.3$; “Ternary systems” counts the Sm-Fe-M systems (of 13) with at least one such entry.

Database	Functional / hull scheme	Entries	Sm-Fe binaries	TbCu_7 family	Ternary systems	Moments exposed
Materials Project [24]	GGA/GGA+U, MP2020 corrections [37]	61	7	35	10 of 13	No (keyless)
AFLOW [25]	PBE	0	0	0	0 of 13	–
JARVIS-DFT [26]	OptB88vdW	14	7	7	0 of 13	Per cell
NOMAD/Alexandria [27,28]	PBE	354	24	75	13 of 13	Per site
OQMD [29,30]	PBE(+U), fitted potentials	191	37	23	5 of 13	No (keyless)
GNoME [31]	PBE, vs. MP+OQMD hull	8	0	2	2 of 13	No

A. Database retrieval

All entries containing Sm and Fe with at most three elements, plus Sm-Co binaries for reference, were retrieved on 13 October 2026 through keyless public interfaces. The OPTIMADE API [38] was used for MP (stability block GGA/GGA+U with the MP2020 correction scheme [37]), JARVIS-DFT, OQMD and Alexandria; the AFLUX API for AFLOW; the NOMAD search API for an inventory of NOMAD-hosted calculations; and the public GNoME summary and $r^2\text{SCAN}$ files (151 MB and 22 MB). Entries containing elements outside $\{\text{Sm}, \text{Fe}, \text{Co}, \text{M}\}$ were discarded. Each database’s own E_{hull} was used, without mixing energies across databases. For GNoME, whose decomposition energy is reported relative to the combined MP+OQMD hull, negative values (predicted stable) were clipped at zero. NOMAD-hosted copies of MP and OQMD data were not double counted. Thermodynamic values for the 451 NOMAD-hosted Alexandria calculations were read from the Alexandria OPTIMADE endpoint, because the NOMAD index does not carry formation energies.

Every raw response is archived with its byte size and SHA-256 digest, and each file was cross-checked against an independent second retrieval, with identical digests over the compared fields [35]. For the 75 Sm-Fe binary entries, the convex hull was recomputed from each database’s formation energies with Eqs. (4)–(5). The recomputed E_{hull} agrees with the value each database

reports to within 2 meV/atom for every entry (largest difference: JARVIS-DFT SmFe_{12}), and no entry differs by more than 5 meV/atom.

B. Structure-family classification

Each entry was assigned a stoichiometry class from its ratio x [Eq. (1)]. Zr and Hf, which commonly occupy rare-earth sites, were placed on the R site when that produced a standard ratio; Ti and Nb were placed on the R site only when the transition-metal-site assignment did not. Cubic cells were excluded, and an Fe + Co fraction of at least 0.6 was required for the TbCu_7 family so that Al- and Si-rich compounds are not counted as magnet phases. The classes are CaCu_5 ($x = 5$), 2:17 ($x = 8.5$), 3:29 ($x = 29/3$), ThMn_{12} ($x = 12$) and other Fe-rich approximants ($5.3 < x < 12.3$). PuNi_3 (3), Ce_2Ni_7 (3.5), MgCu_2 (2) and $\text{Sm}_5\text{Fe}_{17}$ (3.4) were classified separately.

	Co	Ti	V	Zr	Nb	Cu	Si	Ga	Al	Mo	Cr	Mn	Hf
Materials Project	3	2	2	2	–	–	4	4	2	2	5	1	–
OQMD	–	–	–	–	–	1	1	3	1	–	2	–	–
NOMAD / Alexandria	23	4	3	3	2	1	6	3	6	2	5	2	1
JARVIS-DFT	–	–	–	–	–	–	–	–	–	–	–	–	–
AFLOW	–	–	–	–	–	–	–	–	–	–	–	–	–
GNoME	1	–	–	–	–	–	–	–	1	–	–	–	–
Scored observations	1	5	3	4	1	1	2	2	1	1	none	none	none

FIG. 2: Number of TbCu₇-family ternary entries per Sm-Fe-M system in each database (darker = more entries; “–” = none), with the number of scored rapid-solidification or milling observations per system in the bottom row. Cr, Mn and Hf have database entries but no qualifying observation.

C. Literature curation

Candidate studies were identified with about 50 OpenAlex [39] keyword queries and the reference lists of recent papers on TbCu₇-type Sm-Fe [14,23]. Inclusion required (i) a Sm-Fe or Sm-Fe-M alloy with M in the core set (minor Co, B or C additions flagged), (ii) preparation by melt spinning, rapid quenching or mechanical alloying, with or without a subsequent anneal, and (iii) a phase identification stated in the open abstract or title. Each observation records the tested structure family, the outcome (formed or not formed), the phase stoichiometry with its basis (reported, nominal or assumed), magnetic data where reported, and the evidence level. Glass formation, other synthesis routes (for example reduction-diffusion [40]), quinary alloys [41,42] and equilibrium phases already covered by the hull-fidelity test [43] were retained as context but not scored. Appendix A lists all 38 observations.

D. Matching observations to entries

An observation is matched to the lowest- E_{hull} entry of its structure family whose atomic fractions of Sm, Fe and M all lie within ± 0.10 of the observed phase. A binary entry is admissible for a ternary observation when it satisfies the same window, because the databases often contain the binary parent but not the dilute ternary. For TbCu₇ observations the metric is

$$\mathcal{M} = \min \left[\Delta E_{\text{TbCu}_7}(x_{\text{obs}}), \min_{k \in W} E_{\text{hull},k} \right], \quad (12)$$

where W is the set of ternary TbCu₇-family entries within the composition window. We call a match *native* when it is an actual database entry for the observed phase (a binary entry for a binary observation, or a ternary entry or ternary approximant), as opposed to the binary-path model or a binary entry standing in for a ternary.

E. Verdicts and validation metrics

With a formability window τ , a “formed” observation is a *hit* if $\mathcal{M} \leq \tau$ and a *miss* otherwise; a “not formed” observation is a *correct rejection* if $\mathcal{M} > \tau$ and a *false alarm* otherwise. The primary window is $\tau = 50$ meV/atom, with sensitivity checks at 25 and 100 meV/atom. Five metrics summarize each database:

- *Coverage*: the fraction of scored observations for which any prediction exists, and the number with a native entry.
- *Hull fidelity*: the number of the equilibrium Sm–Fe compounds $\text{Sm}_2\text{Fe}_{17}$, SmFe_3 and SmFe_2 with $E_{\text{hull}} \leq 10$ meV/atom.
- *Hit rate*: hits/(hits + misses) among covered “formed” observations.
- *Discrimination*: the spread max–min of E_{hull} across three phases of different experimental fate at nearly the same composition: equilibrium $\text{Sm}_2\text{Fe}_{17}$, metastable TbCu_7 SmFe_9 and SmFe_{12} , which melt spinning does not produce.
- *Moment error*: the relative deviation of the computed Fe moment of TbCu_7 SmFe_9 , [Eq. (11)] from the measured moment scaled to 0 K [Eqs. (9)–(10)].

TABLE III: Energy above hull (meV/atom) of the equilibrium Sm–Fe compounds and the number of Sm–Fe binaries on each database’s hull. “Pass” = $E_{\text{hull}} \leq 10$ meV/atom.

Database	$\text{Sm}_2\text{Fe}_{17}$	SmFe_3	SmFe_2	On hull
Materials Project	22.9 (fail)	7.5 (pass)	22.8 (fail)	0
OQMD	20.0 (fail)	6.0 (pass)	23.0 (fail)	0
NOMAD/Alexandria	19.4 (fail)	5.3 (pass)	22.9 (fail)	0
JARVIS-DFT	51.9 (fail)	no entry	1.2 (pass)	1 (SmFe_5)

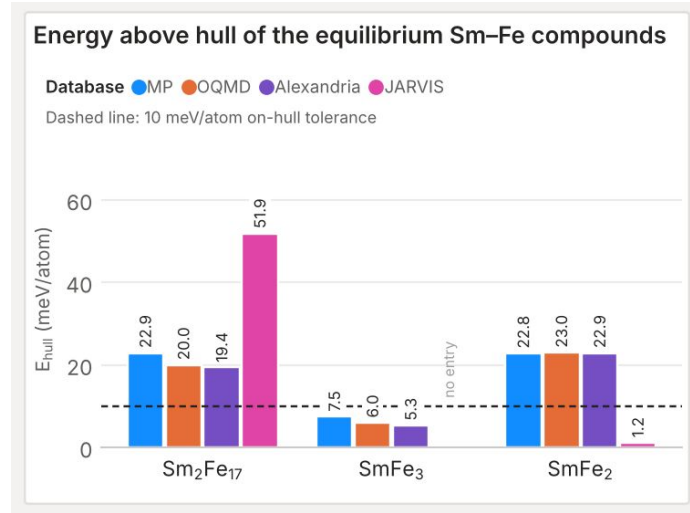


FIG. 3: Energy above hull of the three equilibrium Sm–Fe compounds in each database with Sm–Fe entries. An accurate database would place all three at, or within a few meV/atom of, zero (dashed line: 10 meV/atom tolerance).

F. Reproducibility

The pipeline consists of six numbered Python scripts: retrieval, merging, proxy construction, validation, figures and document generation. All numbers quoted in this paper are written by the pipeline to a single statistics file, and every table in this paper is generated from the archived output files rather than transcribed by hand. Scripts 02–06 rebuild all outputs from the archived raw snapshot without network access [35].

IV. RESULTS

A. Coverage of the Sm–Fe–M space

Figure 1 summarizes the screen. The snapshot contains 628 entries (Table II), and coverage is very uneven. AFLOW holds no Sm–Fe or Sm–Fe–M entry at all; its only Sm–Co entry, MgCu_2 -type SmCo_2 , carries no formation enthalpy. JARVIS-DFT holds seven Sm–Fe binaries and no ternaries in this space. GNoME’s public list, which by construction contains only newly predicted compounds, holds eight entries here, none at an observed composition. Alexandria is the only source with TbCu_7 -family entries in all 13 ternary systems (Fig. 2). On the experimental side, 30 of the 38 curated observations are scorable, in Sm–Fe and ten ternary systems; no qualifying rapid-solidification or milling observation was found for $\text{M} = \text{Cr}, \text{Mn}$ or Hf . The scored observations comprise TbCu_7 formation (14), ThMn_{12} formation (9), 2:17 formation (3), CaCu_5 SmFe_5 (1), $\text{Sm}_5\text{Fe}_{17}$ (1), the hexagonal ω phase of $\text{Sm}_{20}\text{Fe}_{70}\text{Ti}_{10}$ (1), and one case of non-formation, bulk ThMn_{12} SmFe_{12} by melt spinning [22].

B. Hull fidelity in the binary Sm–Fe system

The binary Sm–Fe phase diagram contains three equilibrium compounds, $\text{Sm}_2\text{Fe}_{17}$, SmFe_3 and SmFe_2 , all of which also appear in rapidly quenched alloys of suitable composition [4]. A database that is to guide composition selection should at least place these on, or very near, its convex hull. Table III and Fig. 3 show that MP, OQMD and Alexandria assign positive formation energies to every Sm–Fe binary. Their Sm–Fe hull is therefore simply the line between the elements, and every compound sits above it by approximately its own formation energy: 19.4–22.9 meV/atom for $\text{Sm}_2\text{Fe}_{17}$ and 22.8–23.0 meV/atom for SmFe_2 . The only “passes” in these three databases are for SmFe_3 (5.3–7.5 meV/atom), whose small positive formation energy happens to fall inside the 10 meV/atom tolerance. JARVIS-DFT behaves differently. It gives SmFe_5 a negative formation energy (–29 meV/atom), which places that compound—not an equilibrium phase—on the hull, and it puts SmFe_2 within 1.2 meV/atom of the hull, but it places $\text{Sm}_2\text{Fe}_{17}$ 51.9 meV/atom above it. None of the four databases with Sm–Fe entries reproduces the equilibrium phase constitution of the system. The underlying entries are listed in Appendix B (Table A2).

C. The TbCu_7 stability proxy

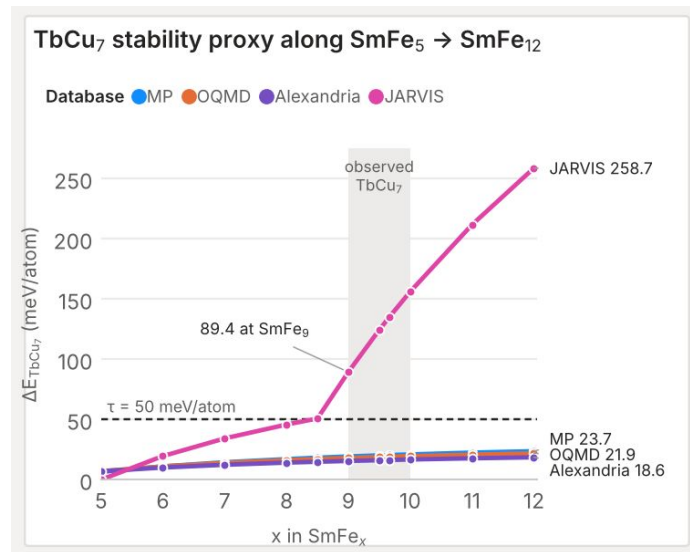


FIG. 4: TbCu_7 stability proxy $\Delta E_{\text{TbCu}_7}(x)$ [Eq. (6)] along $\text{SmFe}_5 \rightarrow \text{SmFe}_{12}$ for the four databases with Sm–Fe entries. The shaded band marks the observed TbCu_7 stoichiometry (SmFe_9 – SmFe_{10}), and the dashed line the 50 meV/atom formability window. AFLOW and GNoME contain no Sm–Fe entries.

TABLE IV: TbCu_7 stability proxy ΔE_{TbCu_7} (meV/atom) along the binary path, with δ from Eq. (2), f from Eq. (3) and the configurational term TS_{conf} at 1273 K from Eq. (7). The last row gives the free-energy proxy of Eq. (8) at the observed composition $x = 9$.

x	δ	f	MP	OQMD	NOMAD/Alexandria	JARVIS-DFT	TS_{conf}
5	0.000	0.8333	6.5	7.1	7.0	0.0	0.0
6	0.125	0.8571	11.1	11.0	10.1	19.6	6.7
7	0.222	0.8750	14.5	14.0	12.4	34.3	9.3
8	0.300	0.8889	17.1	16.3	14.2	45.8	10.6
8.5	0.333	0.8947	18.3	17.2	14.9	50.8	11.0
9	0.364	0.9000	19.3	18.1	15.6	89.4	11.3
9.5	0.391	0.9048	20.2	18.9	16.2	124.4	11.5
10	0.417	0.9091	21.0	19.6	16.8	156.1	11.6
11	0.462	0.9167	22.5	20.8	17.8	211.7	11.7
12	0.500	0.9231	23.7	21.9	18.6	258.7	11.7
ΔG_{TbCu_7} at $x = 9$, 1273 K			8.0	6.8	4.3	78.1	

Figure 4 and Table IV give the proxy of Eq. (6) along the composition path $\text{SmFe}_5 \rightarrow \text{SmFe}_{12}$. For MP, OQMD and Alexandria the envelope of ordered parents is a nearly straight line from SmFe_5 (6.5–7.1 meV/atom) to SmFe_{12} (18.6–23.7 meV/atom). $\text{Sm}_2\text{Fe}_{17}$ lies slightly above that line in all three, so in these databases the equilibrium 2:17 compound does not even contribute to the envelope. At the observed TbCu_7 composition SmFe_9 the proxy is 19.3 meV/atom (MP), 18.1 meV/atom (OQMD) and 15.6 meV/atom (Alexandria). Including the configurational entropy of Eq. (8) at 1273 K lowers these to 8.0, 6.8 and 4.3 meV/atom. In JARVIS-DFT, by contrast, the envelope rises steeply beyond $\text{Sm}_2\text{Fe}_{17}$: the SmFe_9 proxy is 89.4 meV/atom (78.1 meV/atom with entropy), and SmFe_{12} reaches 258.7 meV/atom on the envelope.

D. Discrimination between phases of different experimental fate

TABLE V: Discrimination test: E_{hull} (meV/atom) of three phases with different experimental fates, the spread max–min, and whether the equilibrium phase is ranked below the metastable one.

Database	$\text{Sm}_2\text{Fe}_{17}$ (stable)	TbCu_7 (forms)	SmFe_{12} (does not)	Spread	Order correct
Materials Project	22.9	19.3	23.7	4.4	no
OQMD	20.0	18.1	22.0	3.9	no
NOMAD/Alexandria	19.4	15.6	18.6	3.8	no
JARVIS-DFT	51.9	89.4	260.8	208.9	yes

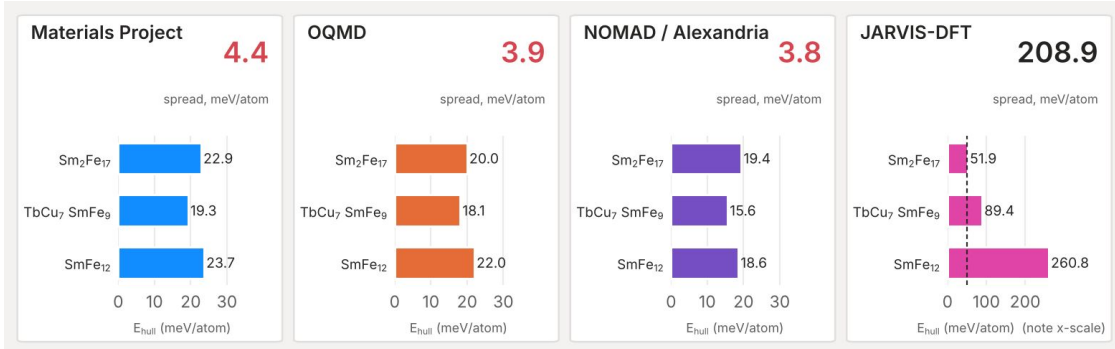


FIG. 5: Energy above hull of equilibrium $\text{Sm}_2\text{Fe}_{17}$, metastable $\text{TbCu}_7 \text{ SmFe}_9$ (proxy) and SmFe_{12} , which melt spinning does not produce, in each database. The number in each panel is the spread between the three phases. A useful descriptor would place $\text{Sm}_2\text{Fe}_{17}$ at zero and separate the three phases by more than the DFT error. Note the different scale for JARVIS-DFT, where the dashed line marks 50 meV/atom.

A screening descriptor is useful only if it separates outcomes that experiment separates. Three Sm–Fe phases at almost the same composition ($f = 0.895$ – 0.923) have three distinct fates. $\text{Sm}_2\text{Fe}_{17}$ is

the equilibrium phase. TbCu_7 SmFe_9 is metastable and forms on rapid quenching [4,8,11]. Bulk SmFe_{12} does not form by melt spinning, which yields an amorphous ribbon [22] or $\text{TbCu}_7 + \alpha\text{-Fe}$ [23]. Table V and Fig. 5 compare the three phases in each database. In MP, OQMD and Alexandria the three energies lie within 4.4, 3.9 and 3.8 meV/atom of one another, respectively—an order of magnitude below typical DFT formation-energy errors—and in all three the metastable TbCu_7 proxy is ranked *below* the equilibrium $\text{Sm}_2\text{Fe}_{17}$. JARVIS-DFT ranks the phases in the experimentally correct order ($\text{Sm}_2\text{Fe}_{17} < \text{TbCu}_7 < \text{SmFe}_{12}$), but its spread of 208.9 meV/atom places the formable TbCu_7 phase well outside any commonly used synthesizability window.

E. Validation against all scored observations

TABLE VI: Database scorecard against the 30 scored observations at $\tau = 50$ meV/atom. “Native” counts observations matched to an actual database entry for the observed phase. Hit rate = hits/(hits + misses). The last two columns give hits/misses at $\tau = 25$ and 100 meV/atom.

Database	With prediction	Native	Hits	Misses	False alarms	Correct rejects	No data	Hit rate	Hits/misses at $\tau =$	
									25 meV	100 meV
Materials Project	25	10	23	1	1	0	5	0.96	21/3	24/0
OQMD	21	3	20	0	1	0	9	1.00	20/0	20/0
NOMAD/ Alexandria	25	9	24	0	1	0	5	1.00	21/3	24/0
JARVIS-DFT	21	3	1	19	0	1	9	0.05	1/19	16/4
AFLOW	0	0	0	0	0	0	30	–	–	–
GNoME	0	0	0	0	0	0	30	–	–	–

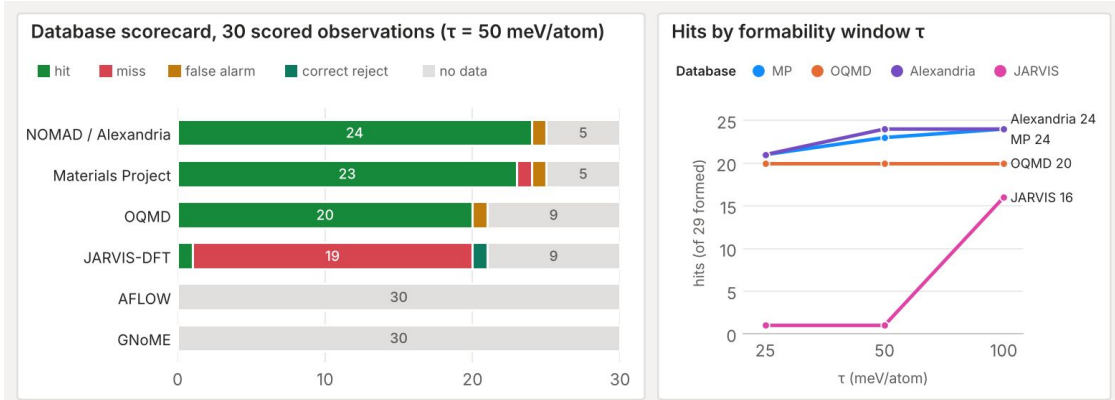


FIG. 6: Left: verdict counts per database at $\tau = 50$ meV/atom. Right: number of hits among the 29 “formed” observations as a function of the formability window τ .

Validation matrix: verdict per observation and database ($\tau = 50$ meV/atom)

Verdict ■ hit ■ miss ■ false alarm ■ correct reject ■ no data Cell value = metric in meV/atom; ^m = binary-path model or binary stand-in

	Materials Project	OQMD	NOMAD / Alexandria	JARVIS-DFT	AFLOW	GNoME
O01 Sm-Fe · TbCu ₇ formed	19.3 ^m hit	18.1 ^m hit	15.6 ^m hit	89.4 ^m miss	no data	no data
O02 Sm-Fe · Th ₂ Zn ₁₇ formed	22.9 hit	20.0 hit	19.4 hit	51.9 miss	no data	no data
O03 Sm-Fe · TbCu ₇ formed	19.3 ^m hit	18.1 ^m hit	15.6 ^m hit	89.4 ^m miss	no data	no data
O04 Sm-Fe · TbCu ₇ formed	19.3 ^m hit	18.1 ^m hit	15.6 ^m hit	89.4 ^m miss	no data	no data
O07 Sm-Fe · Th ₂ Ni ₁₇ formed	22.9 hit	20.0 hit	19.4 hit	51.9 miss	no data	no data
O08 Sm-Fe · TbCu ₇ formed	19.3 ^m hit	18.1 ^m hit	15.6 ^m hit	89.4 ^m miss	no data	no data
O09 Sm-Fe · TbCu ₇ formed	19.3 ^m hit	18.1 ^m hit	15.6 ^m hit	89.4 ^m miss	no data	no data
O10 Sm-Fe · ThMn ₁₂ not formed	23.7 false alarm	22.0 false alarm	18.6 false alarm	260.8 correct reject	no data	no data
O12 Sm-Fe · TbCu ₇ formed	19.3 ^m hit	18.1 ^m hit	15.6 ^m hit	89.4 ^m miss	no data	no data
O13 Sm-Fe-Ti · ThMn ₁₂ formed	15.2 hit	22.0 ^m hit	13.3 hit	260.8 ^m miss	no data	no data
O15 Sm-Fe-Ti · ω phase formed	no data	no data	no data	no data	no data	no data
O16 Sm-Fe-Ti · CaCu ₅ formed	6.5 ^m hit	7.0 ^m hit	7.0 ^m hit	0.0 ^m hit	no data	no data
O17 Sm-Fe-Ti · Sm ₅ Fe ₁₇ formed	no data	no data	no data	no data	no data	no data
O18 Sm-Fe-Ti · ThMn ₁₂ formed	15.2 hit	22.0 ^m hit	13.3 hit	260.8 ^m miss	no data	no data
O19 Sm-Fe-V · ThMn ₁₂ formed	32.0 hit	no data	46.5 hit	no data	no data	no data
O20 Sm-Fe-V · ThMn ₁₂ formed	32.0 hit	no data	46.5 hit	no data	no data	no data
O21 Sm-Fe-V · TbCu ₇ formed	18.4 hit	18.1 ^m hit	15.6 ^m hit	89.4 ^m miss	no data	no data
O22 Sm-Fe-Zr · TbCu ₇ formed	19.3 ^m hit	18.1 ^m hit	15.6 ^m hit	89.4 ^m miss	no data	no data
O23 Sm-Fe-Zr · TbCu ₇ formed	19.3 ^m hit	18.1 ^m hit	15.6 ^m hit	89.4 ^m miss	no data	no data
O24 Sm-Fe-Zr · TbCu ₇ formed	19.3 ^m hit	18.1 ^m hit	15.6 ^m hit	89.4 ^m miss	no data	no data
O25 Sm-Fe-Zr · TbCu ₇ formed	21.0 ^m hit	19.6 ^m hit	16.8 ^m hit	156.1 ^m miss	no data	no data
O28 Sm-Fe-Nb · TbCu ₇ formed	21.0 ^m hit	19.6 ^m hit	16.8 ^m hit	156.1 ^m miss	no data	no data
O29 Sm-Fe-Co · TbCu ₇ formed	19.3 ^m hit	18.1 ^m hit	15.6 ^m hit	89.4 ^m miss	no data	no data
O30 Sm-Fe-Ga · TbCu ₇ formed	19.3 ^m hit	18.1 ^m hit	15.6 ^m hit	89.4 ^m miss	no data	no data
O31 Sm-Fe-Ga · ThMn ₁₂ formed	no data	no data	no data	no data	no data	no data
O32 Sm-Fe-Si · Th ₂ Zn ₁₇ formed	22.9 hit	20.0 hit	19.4 hit	51.9 miss	no data	no data
O33 Sm-Fe-Si · ThMn ₁₂ formed	95.9 miss	no data	39.9 hit	no data	no data	no data
O34 Sm-Fe-Al · ThMn ₁₂ formed	no data	no data	no data	no data	no data	no data
O35 Sm-Fe-Cu · ThMn ₁₂ formed	no data	no data	no data	no data	no data	no data
O36 Sm-Fe-Mo · ThMn ₁₂ formed	12.0 hit	no data	11.3 hit	no data	no data	no data

FIG. 7: Validation matrix at $\tau = 50$ meV/atom. Each cell gives the metric $\mathcal{M}$ [Eq. (12)] in meV/atom and the verdict; a superscript ^m marks verdicts from the binary-path model or a binary stand-in rather than a native entry. Row labels give the observation identifier (Appendix A), the alloy system, the tested structure family and the outcome.

Figure 7 shows the verdict for every scored observation in every database, and Table VI and Fig. 6 summarize them. At $\tau = 50$ meV/atom, Alexandria scores 24 hits, MP 23 and OQMD 20, with at most one miss each. All three, however, also return a false alarm for bulk SmFe₁₂, the only “not formed” observation, because they place it at 18.6–23.7 meV/atom. Given the discrimination result above, these high hit rates reflect a uniformly shallow energy landscape rather than predictive skill: in these databases nearly every Fe-rich Sm-Fe arrangement falls inside the window. JARVIS-DFT scores 1 hit, 19 misses and the single correct rejection. AFLOW and GNoME have no comparable entry for any observation.

Native matches are scarce. MP has native entries for 10 observations, Alexandria for 9, and JARVIS-DFT and OQMD for 3 each; all other verdicts rest on the binary-path model or on a binary entry standing in for a ternary alloy. Five observations have no prediction in any database: the ω phase of Sm₂₀Fe₇₀Ti₁₀ [44], the Sm₅Fe₁₇ phase [45], and the Ga-, Al- and Cu-stabilized ThMn₁₂ alloys [20].

The verdicts depend only weakly on τ for MP, OQMD and Alexandria (Fig. 6, right). Tightening the window to 25 meV/atom turns two MP hits and three Alexandria hits into misses—all of them ternary ThMn₁₂ cases—while leaving the TbCu₇ and false-alarm verdicts unchanged. Widening it to 100 meV/atom raises JARVIS-DFT from 1 to 16 hits. Rejecting SmFe₁₂ while still accepting the formed binary phases would need a window between 22.9 and 23.7 meV/atom in MP (0.8

meV/atom wide) or between 20.0 and 22.0 meV/atom in OQMD, far finer than DFT accuracy; in Alexandria, where SmFe_{12} lies below $\text{Sm}_2\text{Fe}_{17}$, no window does it.

F. Ternary systems

Where native ternary entries exist they behave sensibly (Appendix B, Table A3). $\text{ThMn}_{12}\text{SmFe}_{11}\text{Ti}$ (MP 15.2, Alexandria 13.3 meV/atom), $\text{SmFe}_{11}\text{Mo}$ (12.0, 11.3) and $\text{SmFe}_{10}\text{V}_2$ (32.0, 46.5) all fall inside the window, consistent with their formation in melt-spun and annealed ribbons [20,21,46–48]. The Ti and Mo compounds lie well below binary SmFe_{12} in the same database, reproducing the known stabilizing effect of these elements on the 1:12 structure. MP’s $\text{SmFe}_{10}\text{Si}_2$ (95.9 meV/atom) is the only native miss; Alexandria’s corresponding entry lies at 39.9 meV/atom. MP also contains a V-substituted 2:17 approximant, $\text{Sm}_2\text{Fe}_{16}\text{V}$, at 18.4 meV/atom, which is the matched entry for the Sm–Fe–V TbCu_7 observation.

For the TbCu_7 -forming Zr, Nb and Co additions [5–7,13–15], the binary-path proxy (15.6–21.0 meV/atom in MP, OQMD and Alexandria) is lower than any ternary approximant. The best of these is Alexandria’s R-site-substituted SmZrFe_{10} at 44.7 meV/atom. The databases therefore provide no ternary signal that Zr, Nb or Co stabilizes the TbCu_7 phase, even though this is the best-documented experimental effect in the system.

GNoME’s new predictions in this space are instead R-site-substituted PuNi_3 -type compounds, SmZr_2Fe_9 and SmHf_2Fe_9 , predicted 13.2 and 8.4 meV/atom below the MP+OQMD hull. On $r^2\text{SCAN}$ re-evaluation SmHf_2Fe_9 moves 17.2 meV/atom above that hull. Alexandria finds the same SmM_2Fe_9 family ($M = \text{Zr, Hf, Nb, Ti}$) on its hull. We found no rapid-solidification report of these phases.

G. Fe moments

TABLE VII: Fe moment of $\text{TbCu}_7\text{SmFe}_9$ (μ_B/Fe). Deviations are relative to the midpoint of the 0 K range; the last column gives the interpolation endpoints [Eq. (11)].

Source	m_{Fe}	Dev.	Note
Measured, 293 K (Katter <i>et al.</i>)	1.634	–	–
Measured, scaled to 0 K ($s = 0.3\text{--}0.7$)	1.879–1.955	–	–
NOMAD/Alexandria (computed)	2.228	+16%	SmFe_5 (2.182) / SmFe_{12} (2.244)
JARVIS-DFT (computed)	1.503	–22%	$\text{Sm}_2\text{Fe}_{17}$ (1.36) / SmFe_{12} (2.128)
Materials Project	–	–	moments not exposed (keyless)
OQMD	–	–	moments not exposed (keyless)

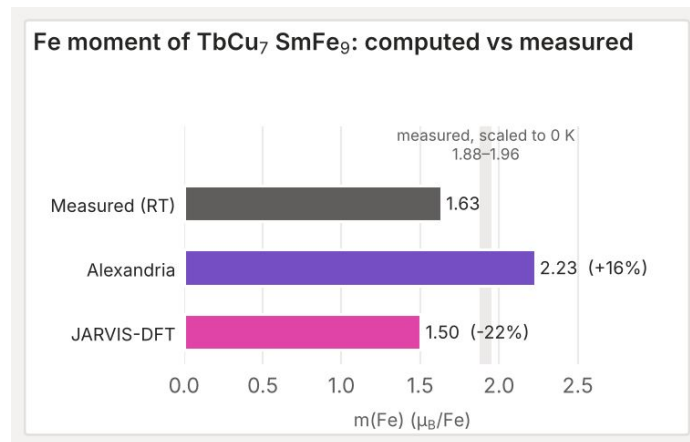


FIG. 8: Average Fe moment of $\text{TbCu}_7\text{SmFe}_9$: measured at 293 K, measured value scaled to 0 K (shaded range), and values interpolated from the two databases that publish moments. Percentages are deviations from the midpoint of the 0 K range.

Katter *et al.* report a saturation polarization of 1.25 T at 293 K for melt-spun $\text{TbCu}_7\text{SmFe}_9$ with $a = 4.88 \text{ \AA}$, $c = 4.23 \text{ \AA}$ and $T_C = 483 \text{ K}$ [4]. Equation (9) gives $V = 87.2 \text{ \AA}^3$ and $m_{\text{Fe}} = 1.63 \mu_B/\text{Fe}$ at 293

K. With $\tau = 0.61$, Eq. (10) scales this to 1.88–1.96 μ_B/Fe at 0 K for $s = 0.3$ –0.7. Interpolating each database’s ordered parents [Eq. (11)] gives 2.23 μ_B/Fe for Alexandria, 16% above the midpoint of that range, and 1.50 μ_B/Fe for JARVIS-DFT, 22% below it (Table VII, Fig. 8). The JARVIS-DFT value is pulled down by an Fe moment of only 1.36 μ_B/Fe in its $\text{Sm}_2\text{Fe}_{17}$ entry, against 2.42 μ_B/Fe in the corresponding Alexandria entry. MP and OQMD do not expose moments through their keyless interfaces. The only moment comparison possible is therefore bracketed by the two databases that report moments, with errors of opposite sign. A second observation, a mixed $\text{TbCu}_7 + \alpha\text{-Fe}$ ribbon at the SmFe_{12} composition with 1.75 μ_B/Fe [23], includes $\alpha\text{-Fe}$ and has no stated measurement temperature, so it is reported but not used for the comparison.

V. DISCUSSION

A. Origin of the flat Sm–Fe energy landscape

The central finding is that three databases fail a basic consistency check: none places the experimentally established equilibrium Sm–Fe compounds on its computed binary convex hull. In their reported datasets, the Fe-rich compounds have small, positive formation energies, and the three phases used in our discrimination test consequently occupy a narrow energy range. One possible explanation is a systematic error in the Sm elemental reference energy. Such an error would shift calculated formation energies in proportion to Sm content [Eq. (4)], potentially contributing to the pattern in Fig. 5. However, the present comparison does not isolate the elemental reference from other sources of error, including exchange–correlation approximations, 4f-electron treatment, magnetic configurations, and incomplete competing-phase coverage. Establishing the cause requires controlled recalculations with consistent references and magnetic states.

The sensitivity to computational choices is illustrated by the different reported energies for SmFe_5 : its $r^2\text{SCAN}$ energy above hull in MP is 50 meV/atom, compared with 6.5 meV/atom in the GGA/GGA+U dataset [49]. This comparison alone does not establish which treatment is more accurate. A useful next step would be to benchmark calculated formation enthalpies and phase rankings against available experimental thermochemistry and known phase equilibria, while testing the effect of elemental-reference corrections [30,37].

B. The JARVIS-DFT case

JARVIS-DFT, which uses the OptB88vdW functional for the entries examined, predicts a markedly steeper energy envelope than the other databases. Its reported Fe moment for $\text{Sm}_2\text{Fe}_{17}$ (1.36 μ_B/Fe) is also substantially smaller than Alexandria’s value (2.42 μ_B/Fe). Differences in magnetic configurations or magnetovolume coupling could contribute to the energy disagreement, but the present data cannot establish whether the JARVIS-DFT state is low-spin, incompletely converged, or simply calculated under different conventions. Resolving this requires matched calculations of the relevant structures with explicit checks of magnetic ordering, volume and convergence. For the current screening test, the consequence is clear: JARVIS-DFT misses 19 of the 20 covered formed observations at the 50 meV/atom threshold.

C. Implications for computational composition screening

For composition selection, the first stage of a computation-guided magnet-development workflow, the findings imply three practical rules.

1. *A low E_{hull} alone is insufficient evidence of formability in Sm–Fe–M.* Within 50 meV/atom, MP, OQMD and Alexandria accept the equilibrium, metastable and non-formable phases alike, so hit rates near 100% here carry no predictive information.
2. *Relative ranking within a database, not absolute E_{hull} , should be screened.* A useful screen would rank TbCu_7 or 2:17 candidates against the competing CaCu_5 , ThMn_{12} and $\alpha\text{-Fe} + 2:17$ assemblages at the same composition. In the present databases even that ranking is wrong for $\text{Sm}_2\text{Fe}_{17}$ versus TbCu_7 SmFe_9 .

3. *Structure coverage limits what can be screened.* No database contains disordered TbCu_7 , the ω phase or $\text{Sm}_5\text{Fe}_{17}$; all but one of the 56 TbCu_7 verdicts in Fig. 7 rest on the proxy, and two observed phases have no prediction at all. The Zr-, Nb- and Co-stabilized TbCu_7 phases have no ternary signal.

The databases did, however, reproduce the stabilizing effect of Ti and Mo on ThMn_{12} (11–15 meV/atom, below binary SmFe_{12} in the same database), and GNoME and Alexandria both predict a family of R-site-substituted SmM_2Fe_9 compounds on the hull. These are concrete, testable leads for rapid-solidification experiments.

D. Recommendations

We recommend that database providers and users first benchmark Sm–Fe phase equilibria and magnetic states before applying a universal energy-above-hull cutoff. Targeted recalculations should test the Sm elemental reference, the 4f-electron treatment and the magnetic configurations of competing structures rather than assuming that any one factor explains the discrepancies. Database coverage would also benefit from explicit disordered TbCu_7 models, for example special quasirandom structures, as well as the experimentally reported ω and $\text{Sm}_5\text{Fe}_{17}$ prototypes. Where possible, magnetic moments and calculation metadata should be made accessible for independent checks. For practical composition screening, an automated hull-fidelity check against known equilibrium phases is a useful first diagnostic, but passing it would not by itself validate predictions of non-equilibrium phase formation.

E. Limitations

The TbCu_7 stability proxy is constructed from the lower convex envelope of available ordered relatives, not from a direct calculation of a chemically disordered TbCu_7 configuration. It should therefore be interpreted as a screening surrogate rather than a rigorous lower bound on the disordered-phase enthalpy: the ordering energies, structural relaxations and configurations sampled by the databases are not sufficient to establish such a bound. The ideal configurational-entropy term (11.3 meV/atom at SmFe_9 and 1273 K) is likewise a model estimate and may overstate the entropy gain if short-range order is present. In addition, the experimental validation is strongly imbalanced: only one of the 30 scored observations records non-formation. Accordingly, the high hit rates cannot establish specificity, balanced accuracy or general predictive discrimination, and the single false alarm should not be treated as a statistically robust estimate of false-positive performance. Structure families were assigned primarily by stoichiometry rather than full structure matching; several observations rely on abstracts or titles, and some use assumed phase compositions (Appendix A). The non-formation result for SmFe_{12} is specific to bulk rapid solidification, since binary SmFe_{12} has been produced as epitaxial films [18]. The Fe-moment comparison relies on one experimental measurement extrapolated from room temperature. Finally, the analysis reflects the public database snapshot of 13 October 2026 [35].

VI. CONCLUDING REMARKS

We compared six public DFT resources with 30 scored literature observations from rapidly solidified and mechanically milled Sm–Fe–M alloys. Materials Project, OQMD and Alexandria place none of the established equilibrium Sm–Fe binary compounds on their reported convex hulls. Their values for equilibrium $\text{Sm}_2\text{Fe}_{17}$, a TbCu_7 SmFe_9 ordered-parent proxy and SmFe_{12} lie within 5 meV/atom, even though these phases have different outcomes under the experimental processing routes considered. Thus, high hit rates at a 50 meV/atom cutoff do not demonstrate an ability to discriminate among those outcomes. JARVIS-DFT preserves the expected ordering in this three-phase comparison, but its TbCu_7 proxy reaches 89.4 meV/atom and it misses 19 of 20 covered formation observations. AFLOW and GNoME provide no comparable predictions for the scored observations. None of the surveyed resources directly represents disordered TbCu_7 , the ω phase or $\text{Sm}_5\text{Fe}_{17}$. The available computed Fe-moment estimates also differ substantially from the experimental extrapolation.

Energy above hull from present public databases should not, on its own, be used to select compositions for metastable Sm–Fe–M magnet phases. A hull-fidelity check against known equilibrium phases, disordered-phase approximants and openly published moments are prerequisites for reliable screening. The stability proxy table, validation matrix and pipeline are released openly to support that work and to allow the test to be repeated as the databases evolve.

DATA AVAILABILITY

The database snapshots, curated observation table, stability proxy table, validation matrix, figures and pipeline code are openly available at [doi:10.5281/zenodo.23456632](https://doi.org/10.5281/zenodo.23456632) [35] (code under the MIT license; data under CC BY 4.0), with the source repository at <https://github.com/johemeeks/tbcu7-stability-screen>.

FUNDING AND CONFLICTS OF INTEREST

This research received no external funding. The author declares no conflicts of interest.

AUTHOR CONTRIBUTIONS

The author performed the analysis and interpretation of the data and wrote the original draft of the manuscript (CRediT roles: formal analysis; writing – original draft).

USE OF AI TOOLS

An AI assistant (Claude, Anthropic) was used in data collection and in text and table editing. All data analysis and interpretation were performed by the author, who reviewed and verified all content and takes full responsibility for the manuscript.

APPENDIX A: CURATED OBSERVATIONS

TABLE A1: All 38 curated observations. “Family” is the structure family tested against the databases; “Scored” marks the 30 observations used in the validation; “Evidence” gives the level of the source used (abstract or title in open metadata). Phase compositions marked as assumed in the dataset are documented there with their basis [35].

ID	System	Sample	Process	Observed phases	Family	Outcome	Scored	Evidence	Ref.
O01	Sm–Fe	Sm _{10.6} Fe _{89.4}	melt spinning (>15 m/s)	TbCu ₇	TbCu ₇	formed	yes	abstract	[4]
O02	Sm–Fe	Sm ₁₂ Fe ₈₈	melt spinning (lower quench rate / higher Sm)	Th ₂ Zn ₁₇	Th ₂ Zn ₁₇	formed	yes	abstract	[4]
O03	Sm–Fe	Sm _{8.7} Fe _{91.3}	melt spinning	TbCu ₇ + α -Fe	TbCu ₇	formed	yes	abstract	[8]
O04	Sm–Fe	Sm _{12.7} Fe _{87.3}	melt spinning	TbCu ₇ + SmFe ₂	TbCu ₇	formed	yes	abstract	[8]
O05	Sm–Fe	Sm _{27.5} Fe _{72.5}	melt spinning	amorphous	amorphous	formed	no	abstract	[8]
O06	Sm–Fe	Sm _{8.7} Fe _{91.3} and Sm _{12.7} Fe _{87.3}	mechanical grinding 72 ks in N ₂	α -Fe + amorphous Fe-Sm	amorphous	formed	no	abstract	[8]
O07	Sm–Fe	Sm-Fe (Sm ₂ Fe ₁₇ target)	mechanical alloying + crystallization anneal	Sm ₂ Fe ₁₇ via metastable intermediate (possibly hexagonal Th ₂ Ni ₁₇ -type)	Th ₂ Ni ₁₇	formed	yes	abstract	[9]
O08	Sm–Fe	Sm-Fe powders	mechanical alloying + annealing	modified TbCu ₇ + Th ₂ Zn ₁₇	TbCu ₇	formed	yes	title	[10]
O09	Sm–Fe	SmFe melt-spun powders	melt spinning	TbCu ₇	TbCu ₇	formed	yes	title	[11]
O10	Sm–Fe	Fe _{92.3} Sm _{7.7} (SmFe ₁₂ stoichiometry)	high-speed melt spinning	amorphous (no bulk ThMn ₁₂ SmFe ₁₂)	ThMn ₁₂	not formed	yes	abstract	[22]
O11	Sm–Fe	SmFe ₂	melt spinning 30 m/s	mostly amorphous + nanocrystalline SmFe ₂	MgCu ₂	formed	no	abstract	[43]
O12	Sm–Fe	SmFe ₁₂ (B-free member of SmFe ₁₂ B _x series)	melt spinning 40 m/s	TbCu ₇ + α -Fe	TbCu ₇	formed	yes	abstract	[23]
O13	Sm–Fe–Ti	SmFe ₁₀ Ti	melt spinning	ThMn ₁₂ (SmFe ₁₁ Ti) + α -Fe	ThMn ₁₂	formed	yes	abstract	[46]
O14	Sm–Fe–Ti	Sm ₂₈ Fe ₆₂ Ti ₁₀	mechanical alloying	multiphase, new hard Sm ₂₃ Fe ₇₃ Ti ₄ phase	other	formed	no	abstract	[46]
O15	Sm–Fe–Ti	Sm ₃₀ Fe ₇₀ Ti ₁₀	melt spinning (crystallized amorphous ribbon)	ω phase (20:70:10)	ω	formed	yes	abstract	[44]
O16	Sm–Fe–Ti	SmFe _{5-x} Ti _x	melt spinning	SmFe ₅ (CaCu ₅) + Sm ₃ Fe ₁₇	CaCu ₅	formed	yes	title	[45]
O17	Sm–Fe–Ti	SmFe _{5-x} Ti _x	melt spinning	Sm ₃ Fe ₁₇ (+ SmFe ₅)	Sm ₃ Fe ₁₇	formed	yes	title	[45]
O18	Sm–Fe–Ti	Sm(Fe,Ti) ₁₂	melt spinning + anneal 750–1050 °C	ThMn ₁₂	ThMn ₁₂	formed	yes	abstract	[20]
O19	Sm–Fe–V	Sm(Fe,V) ₁₂	melt spinning + anneal 750–1050 °C	ThMn ₁₂	ThMn ₁₂	formed	yes	abstract	[20]
O20	Sm–Fe–V	SmFe ₁₀ V ₂	melt spinning	ThMn ₁₂ + α -Fe	ThMn ₁₂	formed	yes	abstract	[48]
O21	Sm–Fe–V	Sm ₁₀ (Fe _{0.95} Co _{0.05}) _{82.5} V _{7.5}	melt spinning 50 m/s	SmFe ₇ -type (TbCu ₇)	TbCu ₇	formed	yes	title, abstract	[12]
O22	Sm–Fe–Zr	low-Sm Sm-Zr-Fe-Co	rapid quenching	TbCu ₇ (SmFe ₇) + α -Fe	TbCu ₇	formed	yes	abstract	[6]
O23	Sm–Fe–Zr	Sm ₈ Zr ₃ Fe ₈₅ Co ₄	melt spinning	TbCu ₇ (SmFe ₇) + α -Fe	TbCu ₇	formed	yes	abstract	[13]
O24	Sm–Fe–Zr	Sm _{8.7} Zr _{1.0} Fe _{85.8} Co _{4.5}	melt spinning 30–40 m/s	single-phase TbCu ₇	TbCu ₇	formed	yes	abstract	[7]
O25	Sm–Fe–Zr	(Sm,Zr)(Fe,Co) ₁₀	rapid quenching	TbCu ₇ (c/a > 0.87)	TbCu ₇	formed	yes	abstract	[5]

ID	System	Sample	Process	Observed phases	Family	Outcome	Scored	Evidence	Ref.
O26	Sm-Fe-Zr	Sm-Zr-Fe	low-temperature reduction-diffusion (600 °C)	TbCu ₇	TbCu ₇	formed	no	abstract	[40]
O27	Sm-Fe-Hf	Sm-Hf-Fe	low-temperature reduction-diffusion (600 °C)	TbCu ₇	TbCu ₇	formed	no	abstract	[40]
O28	Sm-Fe-Nb	SmFe _{10-x} Nb _x ($x = 0.1-0.3$)	melt spinning + anneal	TbCu ₇ (Nb on 2e site), Sm ₂ Fe ₁₇ and α -Fe suppressed	TbCu ₇	formed	yes	abstract	[14]
O29	Sm-Fe-Co	SmFe _{9-x} Co _x ($x = 0, 1, 3, 5$)	melt spinning 12, 20, 32 m/s	TbCu ₇ (as-cast Th ₂ Zn ₁₇)	TbCu ₇	formed	yes	abstract (Chinese)	[15]
O30	Sm-Fe-Ga	Sm _{0.98} Fe _{9.02-x} Ga _x	melt spinning	TbCu ₇	TbCu ₇	formed	yes	title	[16]
O31	Sm-Fe-Ga	Sm(Fe,Ga) ₁₂	melt spinning + anneal 750–1050 °C	ThMn ₁₂	ThMn ₁₂	formed	yes	abstract	[20]
O32	Sm-Fe-Si	Sm ₂ Fe _{17-x} Si _x ($x = 0-2$)	mechanical alloying + anneal	single-phase Th ₂ Zn ₁₇	Th ₂ Zn ₁₇	formed	yes	abstract	[51]
O33	Sm-Fe-Si	Sm(Fe,Si) ₁₂	melt spinning + anneal 750–1050 °C	ThMn ₁₂	ThMn ₁₂	formed	yes	abstract	[20]
O34	Sm-Fe-Al	Sm(Fe,Al) ₁₂	melt spinning + anneal 750–1050 °C	ThMn ₁₂	ThMn ₁₂	formed	yes	abstract	[20]
O35	Sm-Fe-Cu	Sm(Fe,Cu) ₁₂	melt spinning + anneal 750–1050 °C	ThMn ₁₂	ThMn ₁₂	formed	yes	abstract	[20]
O36	Sm-Fe-Mo	Sm(Fe,Mo) ₁₂	melt spinning	ThMn ₁₂	ThMn ₁₂	formed	yes	abstract	[21]
O37	Sm-Fe-Co-Zr-Ti	(Sm _{0.8} Zr _{0.2})(Fe _{0.75} Co _{0.25}) _{11.4} Ti _{0.6}	high-energy milling	amorphous 1:12 + α -Fe/Co	amorphous	formed	no	abstract	[42]
O38	Sm-Fe-Co-Zr-Ti	(Sm _{0.8} Zr _{0.2})(Fe _{0.8} Co _{0.2}) _{11.4} Ti _{0.6}	rapid quenching	ThMn ₁₂ (almost single phase)	ThMn ₁₂	formed	no	abstract	[41]

APPENDIX B: DATABASE ENTRIES BEHIND THE REPORTED VALUES

Tables A2 and A3 list the database entries used for the hull-fidelity test and the native ternary matches, so that each value can be checked against its source record.

TABLE A2: Database entries behind Table III (lowest- E_{hull} entry of each compound).

Database	Sm ₂ Fe ₁₇	SmFe ₃	SmFe ₂
Materials Project	mp-1426	mp-1102187	mp-1729
OQMD	oqmd-4818030	oqmd-4103652	oqmd-4093401
NOMAD/Alexandria	agm005529553	agm002211668	agm003195273
JARVIS-DFT	JVASP-85844	–	JVASP-19950

TABLE A3: Native ternary entries matched to scored observations (E_{hull} in meV/atom, entry identifier in parentheses). OQMD, JARVIS-DFT, AFLOW and GNoME have no native ternary match.

System	Family	Compound	Observations	Materials Project	NOMAD/Alexandria
Sm–Fe–Mo	ThMn ₁₂	SmFe ₁₁ Mo	O36	12.0 (mp-1219069)	11.3 (agm005280486)
Sm–Fe–Si	ThMn ₁₂	SmFe ₁₀ Si ₂	O33	95.9 (mp-1219261)	39.9 (agm005741265)
Sm–Fe–Ti	ThMn ₁₂	SmFe ₁₁ Ti	O13, O18	15.2 (mp-1219022)	13.3 (agm005220819)
Sm–Fe–V	ThMn ₁₂	SmFe ₁₀ V ₂	O19, O20	32.0 (mp-1219210)	46.5 (agm005266931)
Sm–Fe–V	TbCu ₇	Sm ₂ Fe ₁₆ V (2:17)	O21	18.4 (mp-1219218)	–

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