

From 12,800 Candidates to an Experiment-Ready Tungsten–Cuprate Family

A FluxMateria Whitepaper on Computational Prioritization,
Experimental Readiness, and Validation Strategy

12,800+

Candidates

160.3 K

Screening-est. Tc

<24 hrs

Discovery Time

\$21/kg

Est. Cost

Executive Summary

FluxMateria computationally prioritized a novel tungsten-modified calcium–barium–copper-oxide candidate family through a deterministic physics-native inverse-design workflow that moved from broad search to experiment-ready synthesis planning in under 24 hours.

Starting from more than 12,800 generated candidates, the pipeline narrowed the field to a small, interpretable set of fluorine-free leads and controls, with the strongest branch centered on nominal $\text{WCaBaCu}_3\text{O}_7\text{Mo}$.

The leading targets yielded screening-estimated transition temperatures of approximately 158–162 K, with the primary candidate lead at 160.3 K at ambient pressure. These values are computational screening estimates, not experimental measurements.

What distinguishes this discovery is the translation into a falsifiable experimental program: precursor selection, ceramic synthesis window, oxygen-history branching, a nine-pellet DOE matrix, and a repeatability-gated validation standard.

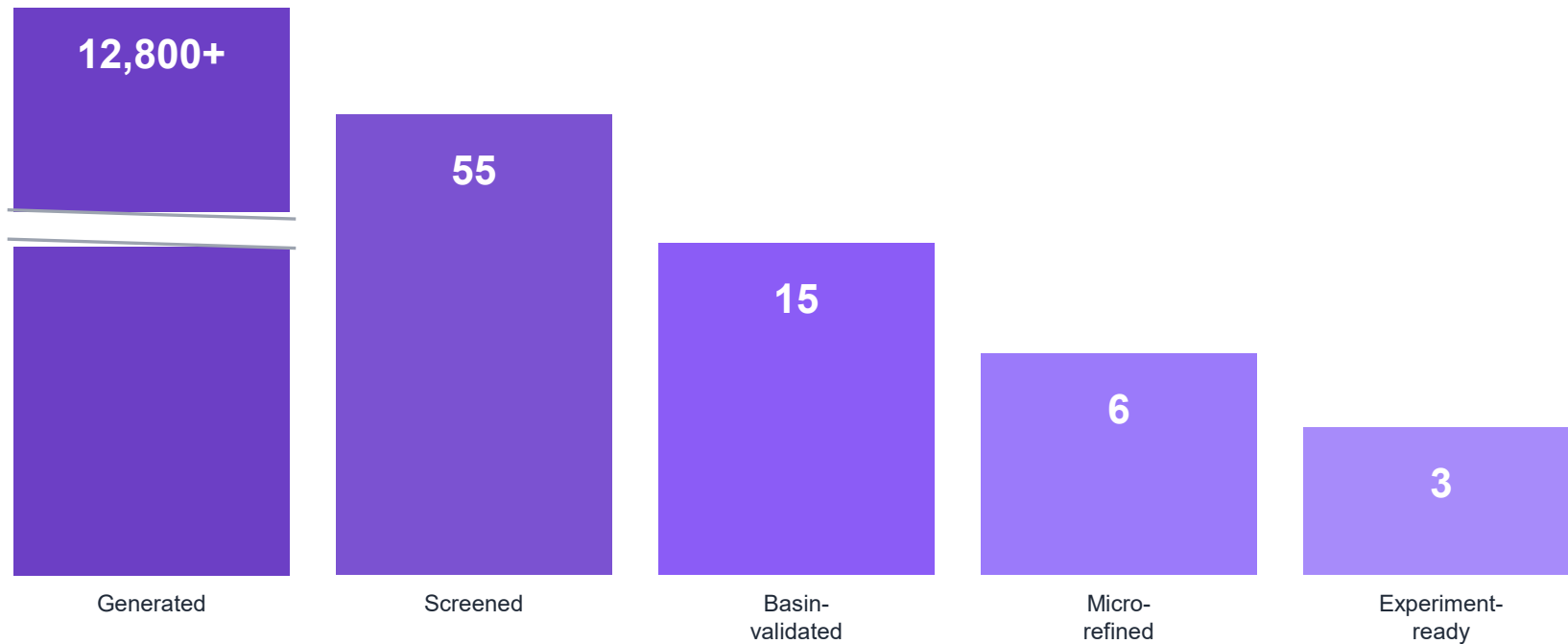
At a Glance

Metric	Result
Generated candidates	12,800+
Passed screening	55
Basin-validated	15
Micro-refined	6
Experiment-ready leads	3
Primary candidate lead	WCaBaCu ₃ O ₇ Mo
Primary screening-estimated Tc	160.3 K
Estimated raw material cost	~\$21.2/kg
Discovery-to-package time	<24 hours
IP status	Patent-pending candidate family

All temperature values shown in this document are computational screening estimates unless explicitly stated otherwise.

Discovery Funnel

The discovery funnel progressively narrowed 12,800+ candidates to 3 experiment-ready leads. Counts reflect computational down-selection stages, not experimental validation.



1. The Problem

High-temperature superconductors remain among the most strategically important classes of materials.

Traditional discovery workflows are slow, expensive, and uncertain:

- Intuition-guided composition selection
- Extensive DFT calculations
- Iterative trial-and-error synthesis
- Under-specified experimental planning

For cuprate-like oxides, nominal composition is rarely the whole story. Oxygen stoichiometry, thermal history, and metastability all matter.

The real challenge is to define a candidate basin and a disciplined way to test it.

2. What FluxMateria Set Out to Test

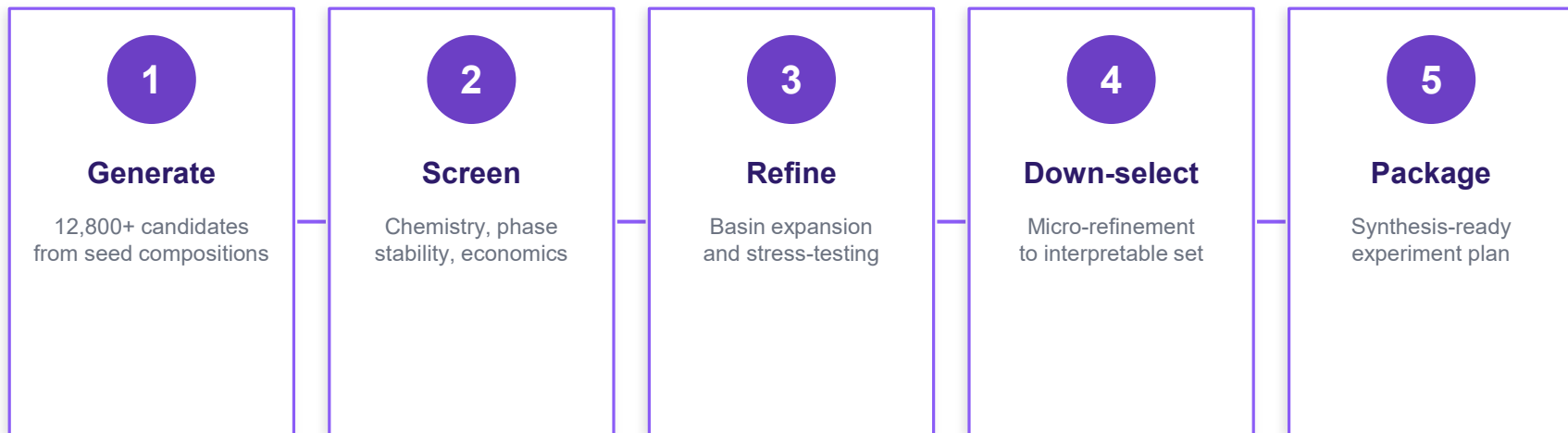
FluxMateria set out to test whether a computational pipeline could identify a novel, practical, ambient-pressure cuprate candidate family with screening-estimated T_c above the mercury-cuprate benchmark, and deliver an experiment-ready validation program in a single research session.

Multi-criteria discovery problem, not a single-objective T_c hunt:

- Superconducting potential
- Chemistry and phase plausibility
- Economics and manufacturability
- Novelty and experimental tractability

The pipeline was designed to output more than rankings — it had to produce a laboratory pathway that could be executed, audited, and falsified.

3. The FluxMateria Discovery Pipeline



Computation becomes a disciplined decision-support system for experimental action.

4. The Disclosed Candidate Family

Nominal general form: $\text{WCaBaCu}_3\text{O}_x\text{M}$, where $x \approx 6-7$ and $\text{M} = \text{Mo}$ or Nb

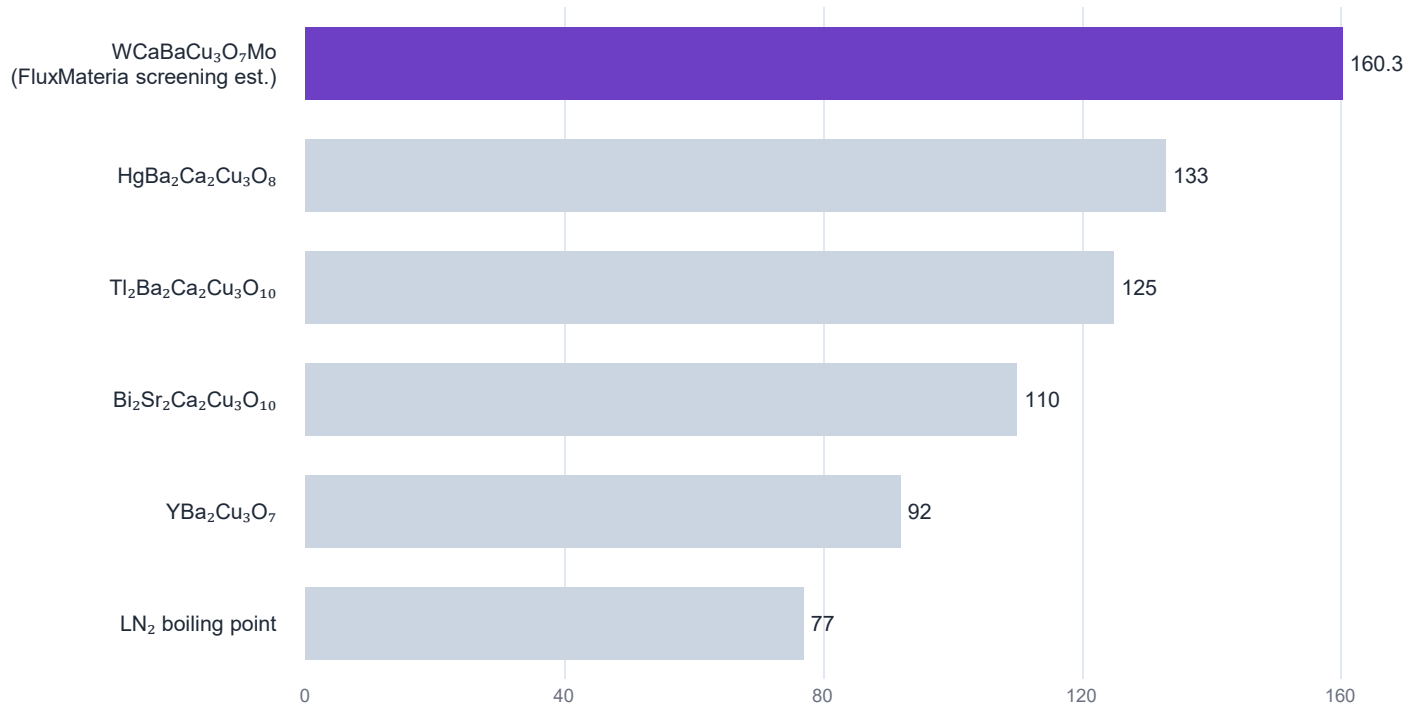
Composition	Role	Screening-est. T_c	Readiness score	Cost/kg
$\text{WCaBaCu}_3\text{O}_7\text{Mo}$	Primary lead	160.3 K	92.5	\$21.2
$\text{WCaBaCu}_3\text{O}_6\text{Mo}$	Same-branch control	160.3 K	92.5	\$21.7
$\text{WCaBaCu}_3\text{O}_6\text{Nb}$	Cross-branch control	158.2 K	92.2	\$25.4
$\text{WCaBaCu}_3\text{O}_7\text{Nb}$	Watchlist variant	158.2 K	92.2	\$25.4

All compositions shown are nominal target formulations for first-pass synthesis planning.

Why the Fluorine-Free Mo Branch Won First Priority:

- High screening-estimated performance
- Stronger experimental tractability
- Lower early-stage interpretive risk
- Easier precursor handling
- More informative lead-control comparisons

Screening Estimate vs. Experimental Benchmarks



Purple = FluxMateria screening estimate for a nominal candidate composition | All others = experimentally measured literature benchmarks

5. Structural Interpretation

Species	Tentative Role
Cu × 3	Mixed-valence Cu ²⁺ /Cu ³⁺ in superconducting CuO ₂ planes
Ba	Charge-reservoir / block layer
Ca	Interlayer spacer between CuO ₂ planes
W	Heavy reservoir dopant / structural stiffener
Mo or Nb	Companion reservoir dopant / valence-tuning modifier

Why Tungsten Is of Interest

To our knowledge, no experimentally verified cuprate superconductor incorporates tungsten as a defining ingredient. W may offer strong electronic/structural influence, high oxidation-state reservoir behavior, abundance relative to Hg-based systems, and non-toxicity.

6. Three-Dimensional Discovery Logic

Composition Space

12,800+ candidates narrowed to 3 fluorine-free leads + controls

Oxygen History

Three explicit oxygen protocols (Rich, Opt, Lean) rather than post-hoc tuning

Pressure History

Contingent Phase 2 pathway: transient pressure conditioning for metastable states

Discovery is reframed from a formula-only problem into a state-and-protocol definition problem.

7. Proposed First-Batch Experimental Program

Precursor System

BaCO₃, CaCO₃, CuO, WO₃
MoO₃ or Nb₂O₅ (branch-dependent)

Process Window

Step	Conditions
Pre-dry	120–180 °C, 2–4 h
1st calcine	760–800 °C, 6–10 h
2nd calcine	840–880 °C, 8–12 h
Sinter	915–945 °C, 10–18 h
Cool-down	O ₂ at ~700 °C

Oxygen-Branch Protocols

Protocol	Conditions
OX-Rich	385–405 °C, 16–20 h, pure O ₂
OX-Opt	425–455 °C, 14–18 h, pure O ₂
OX-Lean	530–560 °C, 10–14 h, 10–15% O ₂ /Ar

Recommended Run Order

1. M1-Opt (primary lead, optimal O₂)
2. M2-Opt (same-branch control)
3. N1-Opt (cross-branch control)

Process windows shown are first-pass protocol targets and may be adjusted based on phase readout and characterization.

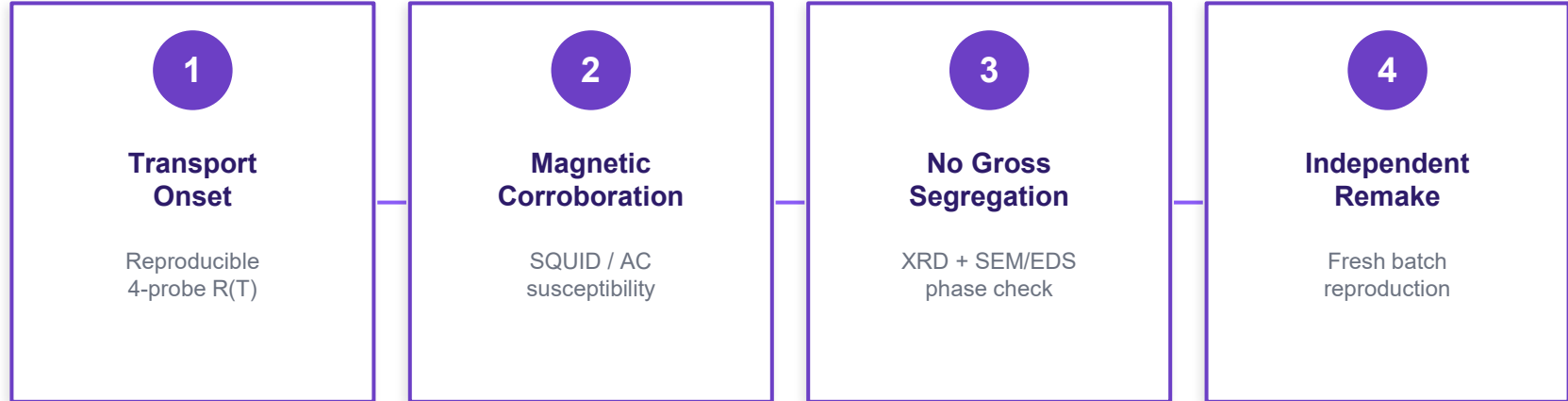
Nine-Pellet First-Batch Screening Matrix

	OX-Rich	OX-Opt	OX-Lean
WCaBaCu ₃ O ₇ Mo	M1-Rich	M1-Opt 1	M1-Lean
WCaBaCu ₃ O ₆ Mo	M2-Rich	M2-Opt 2	M2-Lean
WCaBaCu ₃ O ₆ Nb	N1-Rich	N1-Opt 3	N1-Lean

Highlighted OX-Opt column = recommended first synthesis run. Numbers indicate execution priority.

8. Validation Standard: What Would Count as a Credible Signal

No superconductivity claim should be treated as credible unless all four conditions are met:



Characterization: XRD → SEM/EDS → Four-probe R(T) → SQUID magnetometry

Protects against the most common failure mode: reading too much into a single fragile sample.

9. Why This Matters

Technical Significance

- Candidate tungsten-bearing cuprate family prioritized for first-pass validation
- Screening-estimated ambient-pressure basin above the Hg-cuprate benchmark
- Conventional ceramic route for first-batch testing

Workflow Significance

- Fast narrowing from large search spaces
- Explicit integration of practicality and economics
- Predeclared falsification rules before the first sample is made

Commercial Significance

- Compress full early-stage cycle into actionable package
- Reduce wasted bench effort
- Discovery-to-package in under 24 hours

10. Honest Assessment of Current Status

What Has Been Delivered

- Novel, patent-pending candidate family
- Multi-criteria narrowing across 12,800+ candidates
- Fluorine-free lead-control basin
- Screening-estimated transition-temperature values
- Economics and manufacturability analysis
- First-batch synthesis plan + validation program

What Remains Experimental

- Successful synthesis of target phase
- Crystal structure and oxygen stoichiometry
- Measured transition temperature
- Bulk superconductivity
- Cross-batch reproducibility
- Thin-film or scale-up viability

This distinction is part of the discipline. The value lies in defining a credible path from computation to falsification.

11. Next Milestones

- 1 Execute the three OX-Opt samples in the defined run order
- 2 Perform XRD, SEM/EDS, four-probe R(T), and initial magnetic screening
- 3 Expand oxygen branching only around the most informative signal
- 4 Require fresh-batch remake before treating any anomaly as credible
- 5 Advance only validated fluorine-free winners to pressure-history conditioning
- 6 Use negative or ambiguous results to sharpen the promising boundary

Conclusion

FluxMateria's tungsten–cuprate program is not yet a claim of a confirmed superconductor. At this stage, it is better understood as:

A disciplined discovery-to-validation bridge.

From 12,800+ candidates → novel W-modified calcium–barium–copper-oxide candidate family → fluorine-free Mo lead → complete first-pass experimental framework.

FluxMateria is designed not just to surface interesting materials, but to turn those predictions into disciplined, actionable research programs.

Glossary and Definitions

Sample Codes

Code	Meaning
M1	WCaBaCu ₃ O ₇ Mo (primary lead)
M2	WCaBaCu ₃ O ₆ Mo (same-branch control)
N1	WCaBaCu ₃ O ₆ Nb (cross-branch control)

Oxygen-Anneal Protocols

Protocol	Purpose
OX-Rich	Near-maximum oxygenation / high-hole-doping limit
OX-Opt	Practical optimum balancing O ₂ uptake, ordering, and stability
OX-Lean	Oxygen-deficient underdoped control

Key Terms

Screening-estimated T_c

A computational transition-temperature estimate produced by FluxMateria's physics-native screening pipeline. It reflects the pipeline's ranking of a nominal candidate composition relative to known cuprate families. It is not a measurement, not a DFT prediction, and not a claim of realized performance. Its purpose is prioritization for experimental testing.

Experimental readiness score

A multi-criteria composite score (0–100) reflecting chemistry plausibility, phase stability, manufacturability, economics, novelty, and experiment tractability. Higher scores indicate candidates better suited for immediate first-batch synthesis.