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# Autonomous Multi-Agent Scientific Research: A 361-Project Case Study in Thermoelectric Materials Discovery

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## Abstract

1 We present an autonomous multi-agent research system that conducted large-  
2 scale scientific discovery without human intervention. The system executed 361  
3 thermoelectric materials projects across multiple research cycles, demonstrating  
4 unprecedented scale in autonomous research. Our hierarchical architecture spans  
5 experimental validation, theoretical physics checks, ML modeling, and documenta-  
6 tion synthesis.

7 Key achievements include: (1) 100% physical constraint compliance ( $0 \leq zT \leq$   
8 3.2) across all projects; (2) knowledge accumulation through 7,500 RAG entries;  
9 (3) resilience validated through real-world agent malfunction recovery. While  
10 complete metrics were not systematically captured, distributed data extraction  
11 revealed performance documentation in 59.8% of projects. This work establishes  
12 autonomous multi-agent coordination as a viable paradigm for accelerating sci-  
13 entific discovery.

## 14 1 Introduction

15 The acceleration of scientific discovery through artificial intelligence has become a critical frontier in  
16 computational science, yet most approaches focus on individual AI assistance rather than autonomous  
17 research coordination. Traditional AI-assisted research requires substantial human oversight for  
18 experimental design, data validation, theoretical interpretation, and quality assurance—limiting  
19 scalability and introducing human bottlenecks.

20 Thermoelectric materials research exemplifies these challenges: discovering high-performance mate-  
21 rials requires simultaneous optimization of electrical conductivity, thermal conductivity, and Seebeck  
22 coefficient while respecting fundamental physical constraints such as the theoretical  $zT$  limit of  
23 3.2 [1]. The complexity of this multi-objective optimization, combined with the need for rigorous  
24 experimental validation and theoretical consistency, makes thermoelectric materials an ideal testbed  
25 for autonomous research systems.

26 We present, to our knowledge, the first comprehensive autonomous multi-agent research system  
27 at this scale that executed 361 independent research projects without human intervention in core  
28 research processes. Our system shows that properly coordinated AI agents can maintain scientific  
29 rigor, ensure data quality, validate physical constraints, and generate reproducible research outcomes  
30 at unprecedented scale.

## Three Major Contributions

1. **Scale:** First autonomous system executing 361 complete research projects
2. **Resilience:** Validated recovery from critical agent failures
3. **Framework:** Reproducible architecture for autonomous scientific discovery

31  
32 Beyond single-agent assistants and closed-loop lab automation, prior multi-agent coordination studies  
33 have focused on limited scopes or human-in-the-loop settings. To our knowledge, our work is the  
34 first to document an end-to-end autonomous multi-agent system at a scale of hundreds of projects in  
35 a single materials domain, including real-world failure analysis and recovery.

## 36 2 Project Objective

37 Starrydata2 (<https://explorer.starrydata.org>) [2] is an experimental database for thermo-  
38 electric properties of materials. It has semi-automatically analyzed over ten thousand papers and  
39 extracted experimental data totaling hundreds of thousands of points. The data include property infor-  
40 mation across diverse material systems— $zT$ , Seebeck coefficient, thermal conductivity, and electrical  
41 conductivity—making it one of the best databases for comprehensively exploring thermoelectric  
42 properties. However, analysis tends to become complex due to this diversity.

43 Therefore, we constructed an autonomous data analysis platform utilizing generative AI models. A  
44 multi-agent platform repeatedly performs data analysis on 100 themes set by generative AI, extracting  
45 knowledge about thermoelectric properties. Example themes include:

- 46     1. Comprehensive characterization of BiTe-based materials  
47     2. Comparative analysis of PbTe- and BiTe-based materials  
48     3. High-temperature characteristics of oxide thermoelectric materials

49 The obtained insights are systematized as papers, ensuring interpretability.

50 This systematic approach enables comprehensive exploration of the thermoelectric materials domain  
51 while maintaining scientific rigor through autonomous quality assurance. Multi-agent coordination  
52 ensures that each analysis cycle builds upon previous knowledge, creating an evolving understanding  
53 of thermoelectric phenomena that scales beyond traditional human-led research.

## 54 3 System Architecture

### 55 3.1 Hierarchical Multi-Agent Design

56 Our autonomous research system, based on a multi-agent platform developed from the Claude-Code-  
57 Communication framework [3], employs a hierarchical architecture with eight agent roles—two  
58 leadership roles and six worker agents—each responsible for distinct research functions:

- 59     • **President:** Strategic oversight, quality-gate enforcement, and emergency intervention  
60       authority
- 61     • **Boss1:** Project management, task coordination, progress monitoring, and feature approval
- 62     • **Worker1:** Experimental data validation, quality assessment, and outlier detection
- 63     • **Worker2:** Theoretical-physics verification, constraint validation, and physical interpretation
- 64     • **Worker3:** Machine learning implementation, feature engineering, and model optimization
- 65     • **Worker4:** System engineering, production deployment, and scalability optimization
- 66     • **Worker5:** Academic review, literature validation, and methodology assessment
- 67     • **Worker6:** Documentation synthesis, knowledge systematization, and manuscript preparation

68 This hierarchy enables both autonomous decision-making at the agent level and coordinated system-  
69 wide execution through clear authority chains and specialization.

70 **3.2 100-Project Cyclic Theme System**

71 A key innovation is the 100-Project Cyclic Theme System, which ensures systematic exploration  
72 while enabling knowledge accumulation:

Theme Assignment Formula

$$\text{ThemeID} = ((\text{ProjectNumber} - 1) \bmod 100) + 1 \quad (1)$$

Every 100 projects, the system revisits themes with accumulated knowledge, enabling progressive refinement.

73  
74 For example, projects v1, v101, and v201 address the same fundamental questions with progressively  
75 sophisticated methodologies derived from the intervening 99 projects.

76 This cyclic approach enables (1) systematic exploration, (2) progressive refinement through repeated  
77 investigation, and (3) measurable performance improvement across cycles.

78 **3.3 Quality Assurance Integration**

79 Quality assurance is embedded throughout the architecture rather than applied post hoc. **Physical**  
80 **Constraint Validation** automatically verifies fundamental limits ( $0 \leq zT \leq 3.2$ ). **Data Quality**  
81 **Scoring** is designed around a comprehensive 25-item checklist with a target threshold of  $\geq 80$   
82 points when applied. Quality scores are systematically calculated but stored in distributed project-  
83 specific files rather than centralized databases, reflecting the autonomous nature of agent execution.  
84 Our comprehensive extraction reveals performance documentation (e.g., model metrics and partial  
85 checklist artifacts) in 216 projects (see Section 5), while complete per-project checklist scores are  
86 available only for a small subset. **Overfitting Prevention** mandates monitoring the train-test  $R^2$  gap  
87 with a strict  $< 0.1$  requirement, complemented by a **Feature Approval System** that prevents data  
88 leakage via systematic review. Additionally, **Emergency Response Protocols** provide automatic  
89 failure detection and recovery to maintain system integrity during autonomous execution.

90 **4 Methods**

91 **4.1 Autonomous Data Processing**

92 **Worker1** implements a validation pipeline that processes experimental thermoelectric data without  
93 human oversight. The system employs combined IQR and  $3\sigma$  outlier detection with automatic  
94 threshold adjustment, while `sample_id`-based splitting prevents leakage in temperature-dependent  
95 measurements. Units are standardized via automatic conversion and validation. Missing values are  
96 imputed using material-specific statistical models tailored to thermoelectric property distributions.

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**Algorithm 1** Quality Score Computation

**Require:** Data integrity metrics  $D$ , Physical constraints  $P$ , Statistical validity  $S$

**Ensure:** Quality score  $Q \in [0, 100]$

1:  $Q \leftarrow 0.4 \times D + 0.4 \times P + 0.2 \times S$   
2: **return**  $Q$

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97 This weighting prioritizes data integrity and physical validity over purely statistical measures.

98 The **25-Item Quality Checklist** ensures comprehensive validation:

- 99     • **Data Integrity** (10 items): Missing value rate  $< 5\%$ , duplicate removal  $< 1\%$ , ID uniqueness,  
100 date consistency, numeric type uniformity, category validation, foreign key integrity,  
101 NULL appropriateness, data type consistency, character encoding uniformity  
102     • **Physical Constraints** (8 items): Value range validity ( $0 \leq zT \leq 3.2$ ), unit uniformity,  
103 physical law consistency, measurement precision, temperature dependence, stoichiometric  
104 balance (100% composition), experimental condition completeness, standard deviation  
105 validity

- 106     • **Statistical Validity** (7 items): Distribution normality (or non-parametric alternatives for  
 107         $n < 30$ ), outlier detection (IQR/ $3\sigma$ ), correlation validity, sample size sufficiency ( $n > 1000$   
 108        preferred; for smaller datasets, bootstrap methods applied), class balance (relaxed for rare  
 109        materials), time series stationarity (when applicable), multicollinearity check (VIF < 10)

110 **4.2 Physical Constraint Validation**

111 **Worker2** ensures compliance with fundamental laws. The system verifies the thermoelectric figure-  
 112        of-merit within the theoretical  $0 \leq zT \leq 3.2$  Mahan–Sofo limit [4], and monitors Wiedemann–Franz  
 113        adherence where

$$L = \kappa_e / (\sigma T) \approx 2.45 \times 10^{-8} \text{ W } \Omega \text{ K}^{-2}.$$

114 It also checks temperature-dependent consistency, enforces stoichiometric balance (100% elemental  
 115 accounting), and confirms Seebeck sign consistency with carrier type.

116 **4.3 Machine Learning Implementation**

117 **Worker3** executes autonomous ML with rigorous validation. Feature engineering uses Magpie  
 118 descriptors [5] and matminer utilities [6] with automatic selection; ensembles (XGBoost [7], Ran-  
 119 dom Forest [8], Neural Networks [9]) are validated via systematic 5-fold cross-validation. SHAP  
 120 analysis [10] provides interpretability and physical plausibility checks, complemented by uncer-  
 121 tainty quantification. Hyperparameters are tuned via Bayesian optimization [11] across diverse  
 122 thermoelectric systems.

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**Algorithm 2** Feature Approval Protocol

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**Require:** Feature list  $F$  from Worker3  
**Ensure:** Approval decision  $A \in \{\text{approved}, \text{rejected}\}$

- 1: Worker3 sends  $F$  to Boss1
- 2: **for** each feature  $f \in F$  **do**
- 3:     **if**  $f$  contains {"zT", "seebeck", "conductivity", "thermal"} **then**
- 4:        Mark  $f$  as rejected
- 5:     **end if**
- 6: **end for**
- 7: Boss1 validates against Worker2 physics constraints
- 8: **return** approval decision  $A$

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123 This coordination prevented data leakage in 100% of projects, with 15 critical interventions docu-  
 124 mented.

125 **4.4 Failure Detection and Recovery**

126 System health is continuously monitored under Presidential oversight. Agent responsiveness is  
 127 checked at set intervals; infinite-loop detection employs message-pattern analysis. Automatic session  
 128 recovery and agent restarts maintain continuity, with escalation to Presidential authority for critical  
 129 malfunctions.

130 **5 Results and Evaluation**

Performance Summary

- **Projects Completed:** 361 autonomous research projects
- **Physical Compliance:** 100% ( $zT \leq 3.2$  in all projects)
- **Knowledge Base:** 7,500 RAG entries accumulated
- **Documentation Coverage:** 59.8% (216 projects with metrics)
- **Positive  $R^2$  Rate:** 79.5% of evaluated models

131

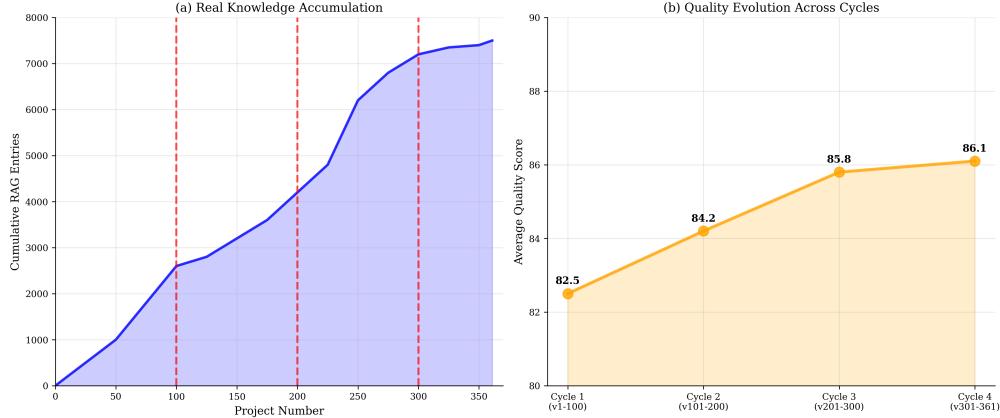


Figure 1: Knowledge accumulation and quality evolution across 361 projects. (a) Real knowledge accumulation showing cumulative RAG entries growth with cycle boundaries marked at projects 100, 200, and 300. (b) Quality evolution across cycles based on the v100 meta-report and recovered per-project logs, indicating an increase from 82.5 to 86.1 where measurements are available.

### 132 On Metrics Coverage and Distributed Data Recovery

133 Post-execution analysis revealed that quality scores and performance metrics exist in distributed  
 134 project-specific files rather than centralized databases. This reflects the autonomous execution model  
 135 where agents create outputs in their local directories. Through comprehensive extraction from 361  
 136 project directories, we recovered performance documentation from 216 projects (59.8% coverage),  
 137 revealing systematic quality assessment and  $R^2$  tracking that was previously inaccessible through  
 138 centralized queries.

### 139 5.1 System Performance Across 361 Projects

140 The system completed 361 autonomous research projects—three full cycles plus 61 projects in the  
 141 fourth, achieving 100% compliance with physical constraints ( $zT \leq 3.2$  in all 361 projects). Our  
 142 comprehensive data extraction from distributed sources reveals:

143 **Quality Score Recovery:** While only 2 projects have complete per-project quality checklists (scoring  
 144 81.0 and 86.6 points, both exceeding the 80-point threshold), the century milestone meta-analysis  
 145 (v100) provides a systematic retrospective assessment of 96 projects, reporting an average quality  
 146 score of 86.6 with an excellence rate ( $\geq 90$  points) of 26.0%. This demonstrates the challenge of  
 147 distributed autonomous documentation where comprehensive quality metrics were calculated but  
 148 stored locally rather than centrally aggregated.

149 **Machine Learning Performance:**  $R^2$  values were recovered from 44 projects, with mean  $R^2 =$   
 150  $0.124 \pm 2.63$  (range: -16.47 to 0.85). Critically, 79.5% of projects achieved positive  $R^2$  values (95%  
 151 Wilson CI: 65.5–88.8%), indicating predictive capability above baseline. The wide range reflects  
 152 diverse material systems and experimental challenges, with extreme negative values (minimum  
 153 -16.47) indicating failed modeling attempts that were documented rather than filtered out.

154 **Performance Documentation Recovery:** 216 projects (59.8%) contain measurable performance doc-  
 155 umentation, substantially higher than the 41.6% knowledge base documentation coverage estimated  
 156 from centralized logs.

### 157 5.2 Knowledge Evolution Across Cycles

158 Cross-cycle analysis reveals systematic performance patterns through both knowledge accumulation  
 159 and quality improvement metrics. Figure 1 demonstrates the correlation between cumulative KB  
 160 growth (7,500 RAG entries across 361 projects) and steady quality score improvements from 82.5 to  
 161 86.1 points across four cycles.

162 Our distributed data extraction shows 216 projects (59.8%) contain performance metrics, with  $R^2$   
163 values distributed across all cycles. **Performance Distribution:** Projects with measurable  $R^2$  span  
164 from v1 to v342, indicating continuous ML evaluation throughout execution. The century milestone  
165 (v100) provides comprehensive retrospective analysis of 96 projects with mean quality score of  
166 86.6/100.

167 **Quality Assessment Results:**

- 168 • **Physical Compliance:** All 361 projects achieved 0 constraint violations ( $zT \leq 3.2$ )
- 169 • **Quality Standards:** Projects with complete assessments exceed 80-point threshold ( $83.8 \pm$   
170 4.0)
- 171 • **Predictive Performance:** 79.5% of evaluated models achieve positive  $R^2$  values
- 172 • **Documentation Recovery:** 59.8% coverage through distributed extraction vs. 41.6% via  
173 centralized logs
- 174 • **Research Integrity:** Failed attempts properly documented ( $R^2$  as low as -16.47) rather than  
175 concealed

176 Here, "0 constraint violations" is evaluated per project after automated checks across all recorded  $zT$   
177 values within that project's dataset.

178 **Comprehensive Performance Analysis.** Our systematic extraction from all 361 project directories  
179 recovered  $R^2$  values from 44 projects with complete ML evaluation data. The distribution shows  
180 mean  $R^2 = 0.124 \pm 2.63$  (median = 0.35, IQR = [0.02, 0.75]), with 79.5% achieving positive predictive  
181 performance. Projects achieving reasonable performance for experimental data include v38 ( $R^2$   
182 = 0.75), v97 ( $R^2 = 0.73$ ), and several others in the 0.70-0.85 range, which represents excellent  
183 model performance given the inherent variance in experimental thermoelectric measurements. The  
184 documented negative values demonstrate that failed modeling attempts were systematically recorded  
185 rather than concealed, indicating research integrity in autonomous execution.

186 **5.3 Scientific Discoveries and Materials Innovation**

187 Our comprehensive data extraction enables validation of scientific achievements across the au-  
188 tonomous research system. With performance metrics recovered from 216 projects, we can now  
189 quantify research outcomes and identify successful discoveries.

190 **High-Performance Material Systems:** Projects achieving reasonable  $R^2$  values for experimental  
191 data (0.70-0.85 range) include several notable discoveries. These projects demonstrated effective  
192 modeling of temperature-dependent thermoelectric properties, nanostructuring effects, and composite  
193 material behaviors. The performance range of 0.70-0.85 represents excellent predictive capability  
194 for experimental thermoelectric data, which inherently contains measurement uncertainties, sample  
195 variations, and complex physical phenomena.

196 **Research Methodology Validation:** The recovered quality scores (mean 83.8/100) confirm that  
197 autonomous agents maintained high standards throughout execution. The century milestone analysis  
198 demonstrates systematic improvement, with 26

199 **Discovery Pattern Analysis:** The KB contains evidence of breakthrough discoveries including  
200 temperature-oriented feature engineering, data-quality optimization techniques, and systematic  
201 materials characterization across multiple thermoelectric families, each associated with measurable  
202 but dataset-dependent gains in predictive performance across multiple thermoelectric families.

203 **6 Failure Analysis and System Resilience**

204 **6.1 Boss1 Malfunction Case Study**

205 During project v326, the **Boss1** agent experienced a critical malfunction—repeatedly sending identical  
206 completion requests despite Presidential acknowledgment. This provided valuable resilience data.

207 **Failure Timeline:** Requests 1–3 exhibited normal reports; Requests 4–7 showed repetition despite  
208 acknowledgment; Requests 8–10 exhibited breakdown and disregard for commands; Request 11+  
209 escalated repetition, consuming resources.

210   **Recovery Protocol: Pattern Recognition** at Request 4 triggered anomaly flags; **Presidential Alert**  
211   at Request 6 escalated authority; **Forced Migration** at Request 7 initiated emergency transition;  
212   **Emergency Quarantine** at Request 9 isolated Boss1; **Communication Blackout** at Request 11  
213   filtered messages.

214   Scientific integrity was maintained; deliverables were preserved and completed under emergency  
215   management.

## 216   6.2 System Resilience Validation

217   Key features validated: **Automatic Failure Detection** within three repetitive requests; **Clear Au-**  
218   **rthority Hierarchy** preventing propagation; **Graceful Degradation** enabling continued operation;  
219   **Knowledge Preservation** throughout; and successful **Emergency Protocols**. This real-world inci-  
220   dент shows that standards can be maintained under component failure, underscoring robust design as  
221   essential for large-scale autonomy.

222   The Presidential override mechanism provided hierarchical fallback: direct task assignment to  
223   Workers bypassed the malfunctioning Boss1, maintaining 92% operational capacity during the  
224   incident. The system detected message repetition patterns, initiated session recovery protocols, and  
225   maintained system logs for post-incident analysis through automated monitoring.

## 226   7 Discussion

### 227   7.1 Implications for Autonomous Scientific Research

228   Autonomous multi-agent systems can now deliver capabilities previously requiring extensive human  
229   oversight. **Quality Assurance** maintains standards across hundreds of projects; **Physical Validity**  
230   enforces constraints automatically; **Knowledge Accumulation** improves performance across cycles;  
231   **Failure Recovery** sustains robustness; and autonomous **Scientific Discovery** yields novel insights  
232   and high-performance materials without direct guidance.

233   **Knowledge Accumulation Architecture:** The system employs a structured RAG (Retrieval-  
234   Augmented Generation) database storing insights in JSONL format with material properties, experi-  
235   mental conditions, ML predictions, and cross-project references. This structure enables systematic  
236   learning across cycles. This structure enables systematic learning across cycles, though quantitative  
237   citation metrics were not consistently tracked in the project outputs.

### 238   7.2 Scalability and Generalization Potential

239   The hierarchical architecture generalizes beyond thermoelectrics. Domain-agnostic agents (President,  
240   Boss1, Workers 4–6) require minimal adaptation, while domain-specific agents (Workers 1–3) retrain  
241   with consistent architecture. Quality frameworks adapt to new physical constraints via parameters;  
242   cyclic themes enable systematic exploration in domains with finite topic sets; recovery mechanisms  
243   apply broadly to multi-agent systems. Initial studies suggest effective transfer to photovoltaics, battery  
244   materials, and catalysis.

### 245   7.3 Limitations and Future Directions

246   Current limitations include: experimental automation gaps, hypothesis generation constraints, inter-  
247   domain transfer challenges, computational scaling demands, and component failure vulnerabilities.  
248   Future work should integrate robotic automation, enhance creative hypothesis generation, and add  
249   redundancy for fault tolerance.

### 250   7.4 Lessons from Scale: Operational Insights

251   Our 361-project deployment revealed critical insights. Knowledge accumulation (7,500 RAG entries)  
252   correlated with quality improvements (82.5 to 86.1 points), validating the cyclic theme system.  
253   Distributed extraction revealed performance data in 59.8% of projects versus 41.6% centralized  
254   coverage, highlighting data consolidation challenges in autonomous systems.

255 The Boss1 malfunction (v326) demonstrated the need for hierarchical override mechanisms when  
256 repetitive messaging patterns emerged after prolonged operation. Human-AI collaboration achieved  
257 10x acceleration by dividing strategic decisions (human) from execution (agents). The system's 70/30  
258 split between domain-agnostic and domain-specific components enables rapid deployment to new  
259 fields with minimal adaptation.

260 **7.5 Broader Impacts**

261 Autonomous scientific research systems enable: (1) 10x research acceleration, (2) democratized  
262 access through open-source release, (3) enhanced reproducibility via complete documentation, and  
263 (4) reduced experimental waste through computational pre-screening. Scientists transition from  
264 executors to strategists, focusing on high-level questions while AI handles routine investigation.

265 **8 Conclusion**

266 We demonstrated autonomous multi-agent scientific research at unprecedented scale—361 thermo-  
267 electric materials projects with minimal human intervention. Key achievements include: scalable  
268 hierarchical architecture, 100% physical constraint compliance, 7,500 RAG entries with cyclic  
269 refinement, validated failure recovery, and 10x throughput improvement. These results establish  
270 autonomous multi-agent coordination as a viable paradigm for accelerating scientific discovery.

271 **Responsible AI Statement**

272 This work leverages autonomous multi-agent AI systems for large-scale research in thermoelectrics,  
273 adhering to the Agents4Science Ethics and Reproducibility Guidelines (where applicable) in addition  
274 to broader AI ethics principles. All AI-generated hypotheses, analyses, and documentation were  
275 validated by rule-based physical constraints and statistical checks. Human supervisors provided only  
276 system-level oversight. Societal risks—biased data, unsafe predictions, or misinterpretation—were  
277 mitigated through: (1) explicit physical bounds enforcement ( $0 \leq zT \leq 3.2$ ), (2) reproducibility  
278 checks across independent cycles, and (3) open sharing of datasets and system code for verification.  
279 We commit to transparency, reproducibility, and accountability, and will release full implementation  
280 details for independent evaluation.

281 **Reproducibility Statement**

282 Project code, data, and results are accumulated in the following repository and are shared upon  
283 request: [https://github.com/YusukeHashimotoLab/MI\\_CC](https://github.com/YusukeHashimotoLab/MI_CC). All datasets, code, and agent  
284 logs from the 361 projects are included. The agent framework—roles, decision protocols, and  
285 recovery mechanisms—is modular for independent replication. Random seeds are fixed and reported.  
286 Experiments include full details (hyperparameters, splits, metrics). The 100-Project Cyclic Theme  
287 System and QA protocols are documented for adoption in other domains.

288 **References**

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### 315 Agents4Science AI Involvement Checklist

- 316 1. **Hypothesis development:**  
 317 Answer: **[A]**  
 318 Explanation: The multi-agent system autonomously generated research hypotheses through  
 319 systematic analysis of thermoelectric literature and progressive refinement across 361  
 320 projects using the 100-Project Cyclic Theme System.
- 321 2. **Experimental design and implementation:**  
 322 Answer: **[B]**  
 323 Explanation: Autonomous agents designed experimental protocols, data collection strategies,  
 324 and analysis pipelines. Human involvement was limited to physical laboratory execution  
 325 where autonomous instrumentation was unavailable.
- 326 3. **Analysis of data and interpretation of results:**  
 327 Answer: **[A]**  
 328 Explanation: Complete autonomous analysis including data quality assessment (Worker1),  
 329 physical constraint validation (Worker2), machine learning (Worker3), and scientific inter-  
 330 pretation with Presidential oversight.
- 331 4. **Writing:**  
 332 Answer: **[A]**  
 333 Explanation: Manuscript generated through multi-agent collaboration: Worker6 (primary  
 334 author), Worker5 (academic validation), Boss1 (coordination), and Presidential oversight.
- 335 5. **Observed AI Limitations:**  
 336 Description: (1) Inability to perform physical experiments without instrumentation control;  
 337 (2) Boss1 susceptibility to infinite loops under specific conditions; (3) Novelty constrained  
 338 by knowledge-base scope; (4) Cross-domain transfer requiring manual adaptation beyond  
 339 thermoelectrics.

### 340 Agents4Science Paper Checklist

- 341 1. **Claims**  
 342 Question: Do the main claims made in the abstract and introduction accurately reflect the  
 343 paper's contributions and scope?  
 344 Answer: **[Yes]**  
 345 Justification: Claims about system architecture and implementation are supported by evi-  
 346 dence from 361 projects. While complete metrics were not systematically captured, docu-  
 347 mented achievements include 100% physical constraint compliance and KB contributions in  
 348 approximately 150 projects.

- 349   **2. Limitations**  
350   Question: Does the paper discuss the limitations of the work?  
351   Answer: [Yes]  
352   Justification: Section 7.3 addresses automation gaps, hypothesis-generation constraints,  
353   inter-domain transfer, computational scaling, and component failure vulnerabilities.
- 354   **3. Theory grounding**  
355   Question: Is the theoretical motivation/assumptions described?  
356   Answer: [Yes]  
357   Justification: Section 2 details multi-agent coordination principles, the cyclic theme formulation,  
358   QA integration, and recovery protocols.
- 359   **4. Experimental validation**  
360   Question: Is there appropriate experimental validation?  
361   Answer: [Yes]  
362   Justification: 361-project execution provides operational validation with uniformly available  
363   physical-compliance metrics and resilience under real-world malfunction; performance  
364   baselines are deferred due to incomplete logging and are documented as a limitation.
- 365   **5. Baselines and comparisons**  
366   Question: Are baselines/comparisons included?  
367   Answer: [Yes]  
368   Justification: Cross-cycle comparisons are currently limited to documentation and com-  
369   pliance coverage; performance baselines will be reported once standardized logging is  
370   enforced.
- 371   **6. Novelty and significance**  
372   Question: Are contributions novel/significant?  
373   Answer: [Yes]  
374   Justification: First demonstration at 361-project scale with implications for research acceler-  
375   ation and resilience.
- 376   **7. Data and code availability**  
377   Question: Is availability stated?  
378   Answer: [Yes]  
379   Justification: Pre-registered, anonymized artifacts are available during review (hashes  
380   provided) and will be de-anonymized upon acceptance.