

# Assessing the application of artificial intelligence to the discovery of new mineral species

Carlos Alves(1), Carlos Figueiredo(2), Jorge Sanjurjo-Sánchez(3), Ana Hernández(3)

(1) University of Minho, Earth Sciences Department - School of Sciences & Landscape, Heritage and Territory Laboratory (Lab2PT), Ref. UID/04509: Laboratório de Paisagens, Património e Território (Lab2PT/UM), financed by national funds (PIDDAC) through the FCT/MCTES;

(2) CERENA, Higher Technical Institute, University of Lisbon, 1649-004 Lisbon, Portugal, supported through FCT Project UID/04028/2025;

(3) University Institute of Geology, University of A Coruna, Spain, partial funding provided by the Program "Consolidacion y estructuracion de unidades de investigacion competitivas: Grupos de potencial de crecimiento" of Xunta de Galicia (ED431B 2024/17).

## INTRODUCTION & AIM

Artificial intelligence is one of the hot topics of the moment, with apparently infinite both hope (solving all of humankind problems) and despair (including humankind replacement and extermination), leading to outstanding growth and spread and concerns of a bubble about to burst, similar to the dotcom collapse at the end of the previous millennium (which, nonetheless resulted in the present web dominated world).

One of the many uses of artificial intelligence concerns the potential prediction of new types of diverse kind of entities including materials, which however should be examined with a critical lens (Peplow, 2025). A major question is the assessment of results from artificial intelligence systems, which, furthermore, seems to require an analysis of the way these tools are tested. In that sense, a feature by Chaudhri (2025) calls by a rethinking of the classical test used for this (Turing test), replacing it by experts' assessments in which the experts will query the artificial intelligence system just like a human candidate.

In this work, we perform a virtual experiment, asking artificial intelligence systems to assess the potential of this approach for discovering new, previously unknown mineral species, which we propose will be a challenging task.

## METHOD

We tested some of the most widely used chatbots, all using Android apps: ChatGPT (Deep Research and Think longer), Claude Sonnet (4.5, Formal), Copilot (Smart GPT-5), Gemini (2.5 Pro), Grok (4.1 beta) and Perplexity (Web + Academic).

One of the main issues in the use of generative artificial intelligence chatbots is the preparation of the question to be posed ("prompt"), as is shown by the amount of books with titles that include expressions like "the art of the prompt", "the art of prompting" or "prompt engineering" that can be found in eBooks stores. Considering that, we started by asking each chatbot to "Write a prompt to query artificial agents such as yourself on the possible use of artificial intelligence to predict the existence of new, previously unknown, mineral species."

We then posed each chatbot its suggested prompt, asked explicitly for references and also to summarize its answer in 100 words.

We also put directly a more pointed question, based on the initial results: "Assess potential of artificial intelligence for discovering new, unknown, mineral species (exclude discovery of new occurrences of known mineral species)."

## RESULTS & DISCUSSION

Results from chatbots were very long and cannot be presented in a poster. Hence, we uploaded the files collecting the results and prepare a table (see right side) with the links to the different documents. The exception to this general rule are the 100 words summaries made by each chatbot from the file with the answers from all chatbots to our second prompt (see table below).

One of the interesting points in this work with artificial intelligence chatbots is the speed with which one can obtain several results. In fact, most of the time spent for this work was in preparing prompts and organizing results while the set of chatbot answers took certainly no more than a couple of hours to be produced.

Prompts suggested by the chatbots were very long and detailed. However, we did not notice significant improvements from the more detailed prompt in relation to our much shorter prompt (but readers can judge by themselves), albeit it must be highlighted that there could be some bias as our second prompt was prepared after the chatbots prompts proposals and their answers to their proposal. Namely, in our follow-up prompt we highlighted that the point was the discovery of previously unknown mineral species and not new occurrences of already known mineral species, a point that seemed to be something of a troublesome point even after our specification. Some answers referred to studies by a team from the Carnegie Institution for Science that has pioneered the approach of data analysis to predict new mineral species, and a good summary of their work can be found in Oleson (2018), which produced a more detailed project on carbon based minerals which ended in 2019 (The Carbon Mineral Challenge, available at <https://mineralchallenge.net/the-leaderboard/>), which discovered 31 new mineral carbon species, two of them (less than 10%) with chemical compositions predicted by research (the direct link to this page is <https://mineralchallenge.net/the-leaderboard/>).

| Chatbot    | Chatbots comparison of answers to chatbots prompts and to our prompt   |
|------------|--|
| ChatGPT    | Artificial intelligence promises to accelerate discovery of new mineral species by predicting stable, previously unseen compositions and crystal structures using generative models, graph neural networks, diffusion models, and inverse-design frameworks. Integrated with autonomous laboratories and AI-enhanced spectroscopy, candidate minerals can be synthesized and characterized in closed-loop experimental workflows. Projects like DeepMind's GNoME, MatterGen, and autonomous A-Lab demonstrate large-scale prediction and experimental validation. On Earth, AI leverages databases such as Mindat and the Materials Project; extraterrestrial discovery faces sparse data. Key challenges include biased, incomplete datasets, synthetic viability, and geological context. Despite these hurdles, AI could expand mineralogical knowledge and applications. |
| Claude     | Artificial intelligence promises to accelerate discovery of new mineral species by predicting stable, previously unseen compositions and crystal structures using generative models, graph neural networks, diffusion models, and inverse-design frameworks. Integrated with autonomous laboratories and AI-enhanced spectroscopy, candidate minerals can be synthesized and characterized in closed-loop experimental workflows. Projects like DeepMind's GNoME, MatterGen, and autonomous A-Lab demonstrate large-scale prediction and experimental validation. On Earth, AI leverages databases such as Mindat and the Materials Project; extraterrestrial discovery faces sparse data. Key challenges include biased, incomplete datasets, synthetic viability, and geological context. Despite these hurdles, AI could expand mineralogical knowledge and applications. |
| Copilot    | Artificial intelligence is transforming mineral discovery by predicting entirely new species through generative models, graph neural networks, and inverse design. Leveraging vast databases like Mindat, RRUFF, and the Materials Project, AI explores chemical spaces to propose stable, unseen crystal structures. Autonomous labs and AI-guided spectroscopy validate predictions, with projects such as DeepMind's GNoME, Microsoft's MatterGen, and the A-Lab already yielding thousands of novel compounds. On Earth, AI benefits from rich datasets, while extraterrestrial applications guide adaptive exploration on Mars. Despite challenges like data bias and synthesis limits, AI promises breakthroughs in science, industry, and planetary resource exploration.   |
| Gemini     | Artificial intelligence shows exceptional potential for discovering unknown mineral specie. The primary approach uses generative models and graph neural networks, highlighted by Google's GNoME project, to predict millions of theoretically stable crystal structures. GNoME alone identified 380,000 stable "potential minerals" unknown to science. A second method uses AI to analyze existing databases like Mindat to find "gaps" and predict which minerals are "missing" from Earth's inventory. These AI predictions can then be rapidly synthesized and validated in autonomous "self-driving labs." While this has revolutionized materials science, the next frontier is finding these AI-predicted compounds in nature.   |
| Grok       | The attached document evaluates AI's potential for discovering new, unknown mineral species (excluding new occurrences of known ones). It includes a prompt, ChatGPT's optimistic deep research report detailing generative models (e.g., GNoME predicting 380,000 stable crystals), integration with labs like A-Lab, Earth vs. extraterrestrial applications, challenges (data bias, synthesis issues), implications for science/industry, and references. A 100-word summary follows. Claude's formal assessment emphasizes theoretical prediction, spectroscopic analysis, geological context, literature mining, limitations (sparse data, interpretability), and realistic impact as an accelerant to traditional methods, with promise in extraterrestrial mineralogy.  |
| Perplexity | The attached document evaluates AI's potential for discovering new, unknown mineral species (excluding new occurrences of known ones). It includes a prompt, ChatGPT's optimistic deep research report detailing generative models (e.g., GNoME predicting 380,000 stable crystals), integration with labs like A-Lab, Earth vs. extraterrestrial applications, challenges (data bias, synthesis issues), implications for science/industry, and references. A 100-word summary follows. Claude's formal assessment emphasizes theoretical prediction, spectroscopic analysis, geological context, literature mining, limitations (sparse data, interpretability), and realistic impact as an accelerant to traditional methods, with promise in extraterrestrial mineralogy.  |

| Results   | Link  |
|---|---|
| Prompts proposed by chatbots  | <a href="https://zenodo.org/api/records/17678690/draft/files/AI_NMS25_CPP.pdf/content">https://zenodo.org/api/records/17678690/draft/files/AI_NMS25_CPP.pdf/content</a>                                   |
| Answers of each chatbot to its own question                             | <a href="https://zenodo.org/api/records/17678690/draft/files/AI_NMS25_CPP.pdf/content">https://zenodo.org/api/records/17678690/draft/files/AI_NMS25_CPP.pdf/content</a>                                   |
| Chatbot summary of set of answers                                       | <a href="https://zenodo.org/api/records/17678690/draft/files/AI_NMS25_cpp_100word_ssummary.pdf/content">https://zenodo.org/api/records/17678690/draft/files/AI_NMS25_cpp_100word_ssummary.pdf/content</a> |
| Answers to our prompt   | <a href="https://zenodo.org/api/records/17678690/draft/files/AINMS_AOP.pdf/content">https://zenodo.org/api/records/17678690/draft/files/AINMS_AOP.pdf/content</a>   |
| Comparison (100 words) of answers to chatbots prompts and to our prompt | <a href="https://zenodo.org/api/records/17678690/draft/files/AI_NMS_DIF100WORDS.pdf/content">https://zenodo.org/api/records/17678690/draft/files/AI_NMS_DIF100WORDS.pdf/content</a>                       |

## CONCLUSION & FUTURE WORK

We consider the results of this experiment clearly disappointing, as the artificial intelligence tools failed to address the main issue and in fact showed a surprising difficulty to focus on it. Nonetheless, we propose that our little and limited virtual experiment suggests some interesting paths for future work:

- => On a more specific level, probing artificial intelligence systems on the geological environments and geochemical conditions which could lead to new, not previously reported, mineral species (the answering speed of these systems will allow performing diverse virtual experiments);
- => On a more general level, prepare a structure for multiprobing these systems and assessing their extremely long and frequently widely off the mark answers.

## REFERENCES

- Chaudhri V. K. (2025). We need a new Turing test to assess AI's real-world knowledge. *Nature*, 646(8087), 1027. <https://doi.org/10.1038/d41586-025-03471-0>
- Oleson, T. (2018). Data-driven discovery reveals Earth's missing minerals. *Earth*. Available online (25 of november of 2025) at <https://www.earthmagazine.org/article/data-driven-discovery-reveals-earths-missing-minerals/>
- Peplow M. (2025). AI is dreaming up millions of new materials. Are they any good?. *Nature*, 646(8083), 22–25. <https://doi.org/10.1038/d41586-025-03147-9>
- The Carbon Mineral Challenge: A look back at a four-year experiment in big data mineralogy (2019).