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A Practical Guide to Building with LLMs

NIST AIMS workshop / July 2024 / Eddie Kim

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About Cohere

2019

Founded

350+

Employees

4 offices

San Francisco, London,
Toronto, New York

Business Partners & Investors

Partners

- ORACLE
- salesforce
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Select Investors

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- ORACLE
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- Jasper
- bambooHR
- LIVEPERSON
- HyperWrite

About me

Manager of Technical Staff @ **Cohere,**
leading our synthetic data research team

Adjunct Prof @ **U of Toronto** in Materials
Science & Engineering

Previously at Xero (fintech + MLops),
Citrine (materials + active learning),
Pfizer (NLP + health), MIT (NLP for materials)

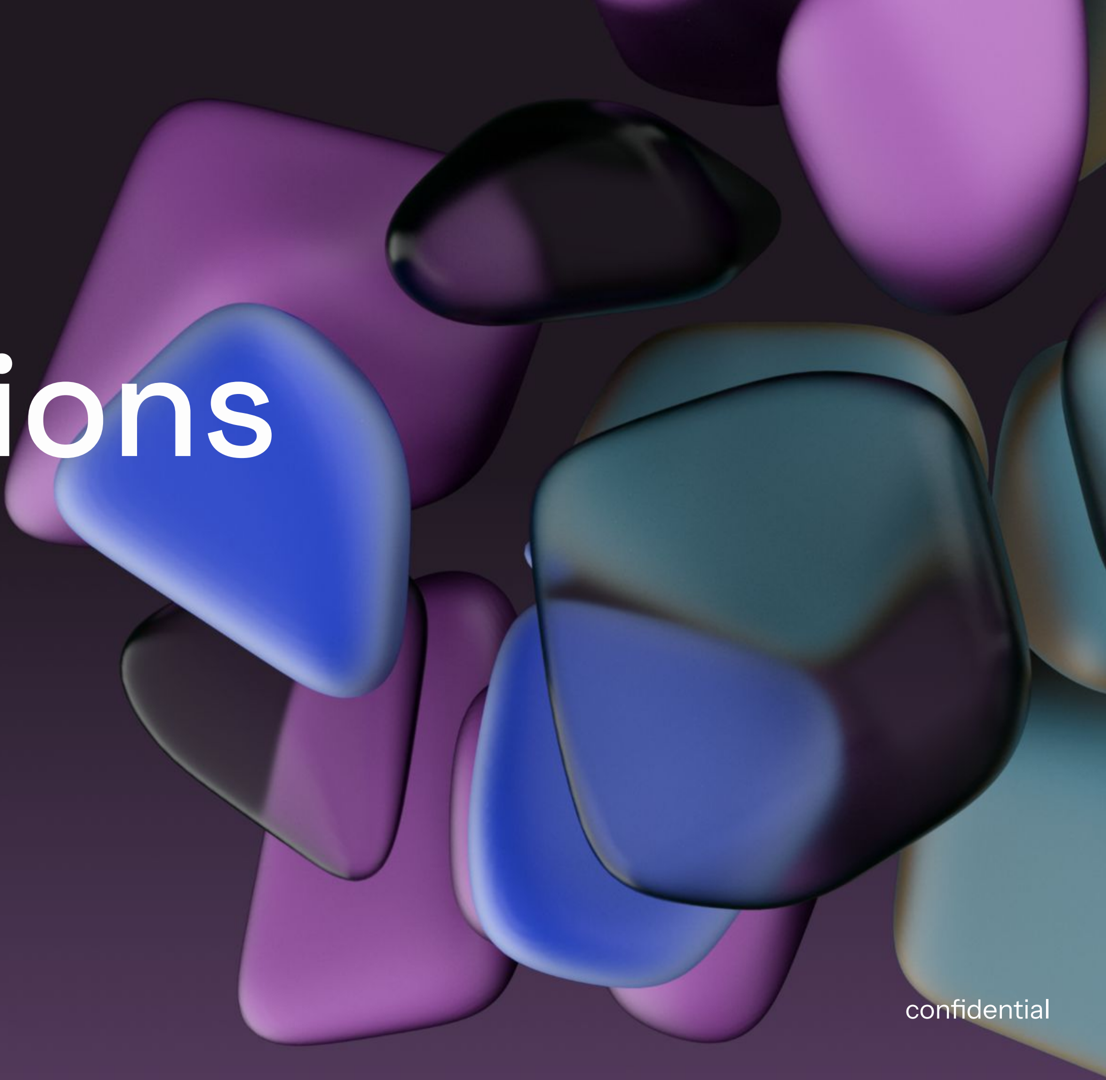
Agenda

01 Core intuitions

02 Failure modes

03 Speculation

Core intuitions



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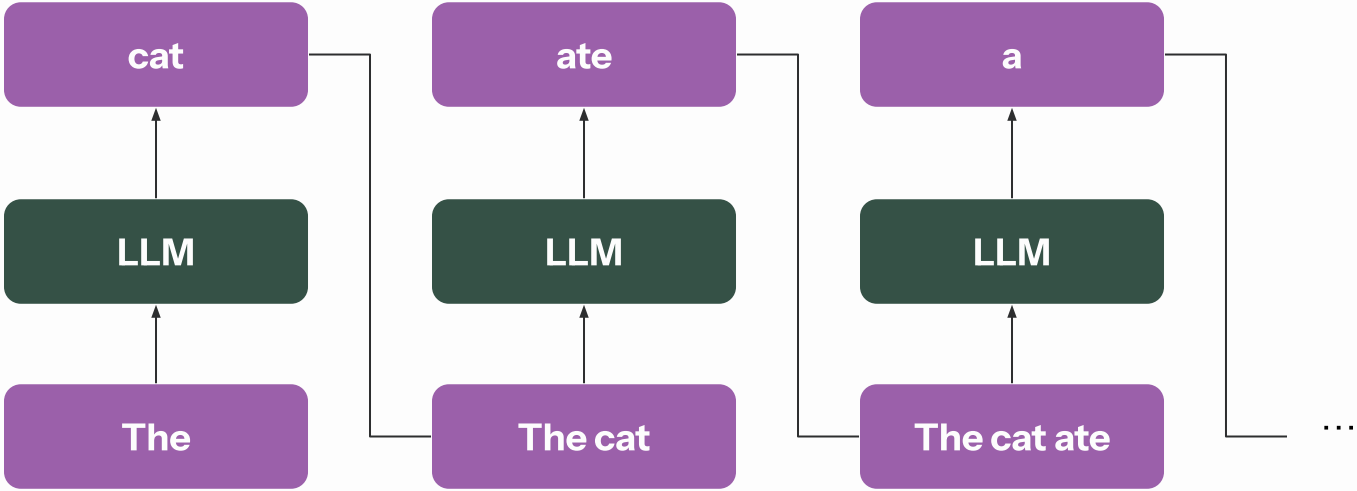
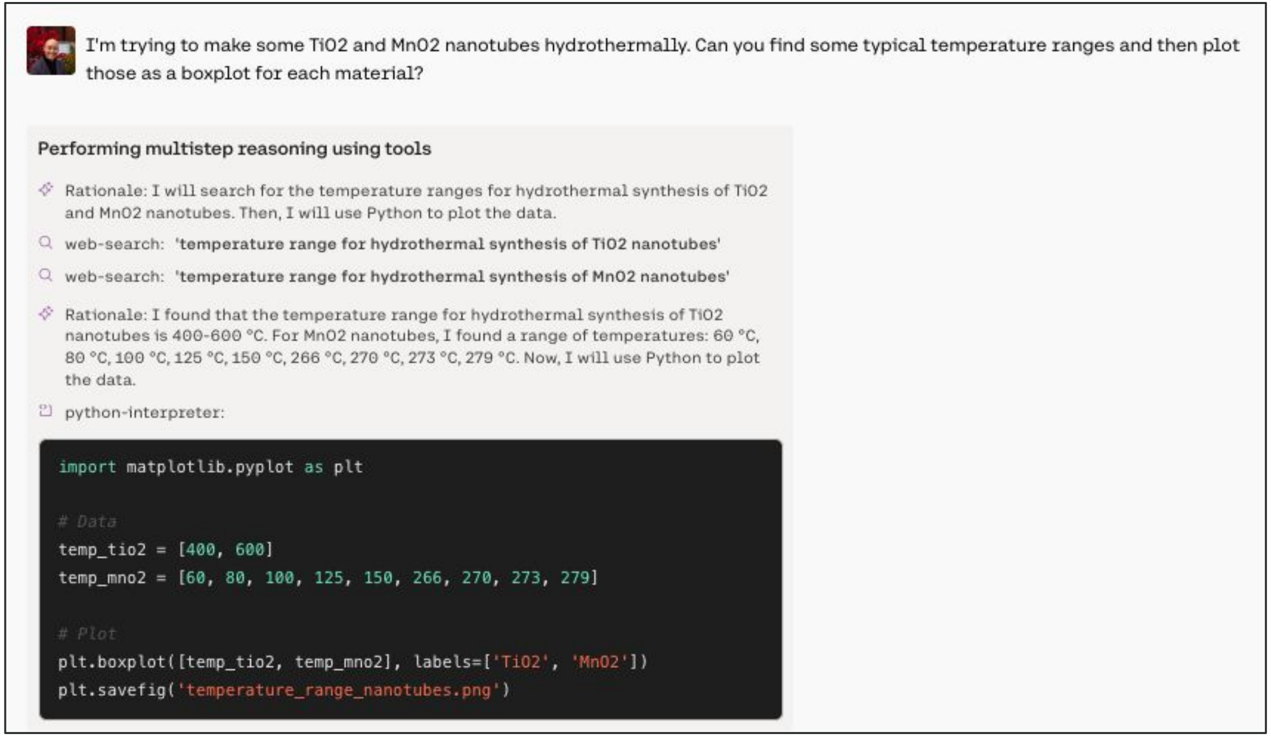
The most important intuition: order matters



Are LLMs useful assistants for materials science?



I'm trying to make some TiO2 and MnO2 nanotubes hydrothermally. Can you find some typical temperature ranges and then plot those as a boxplot for each material?

Performing multistep reasoning using tools

Rationale: I will search for the temperature ranges for hydrothermal synthesis of TiO2 and MnO2 nanotubes. Then, I will use Python to plot the data.

web-search: **'temperature range for hydrothermal synthesis of TiO2 nanotubes'**

web-search: **'temperature range for hydrothermal synthesis of MnO2 nanotubes'**

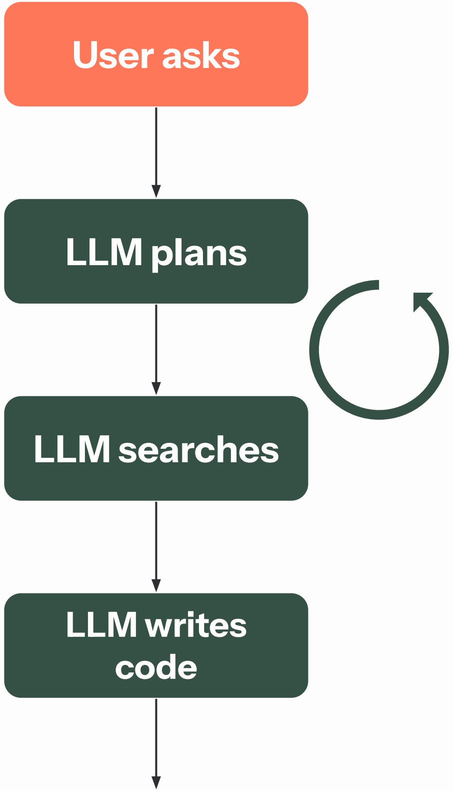
Rationale: I found that the temperature range for hydrothermal synthesis of TiO2 nanotubes is 400-600 °C. For MnO2 nanotubes, I found a range of temperatures: 60 °C, 80 °C, 100 °C, 125 °C, 150 °C, 266 °C, 270 °C, 273 °C, 279 °C. Now, I will use Python to plot the data.

python-interpreter:

```
import matplotlib.pyplot as plt

# Data
temp_tio2 = [400, 600]
temp_mno2 = [60, 80, 100, 125, 150, 266, 270, 273, 279]

# Plot
plt.boxplot([temp_tio2, temp_mno2], labels=['TiO2', 'MnO2'])
plt.savefig('temperature_range_nanotubes.png')
```



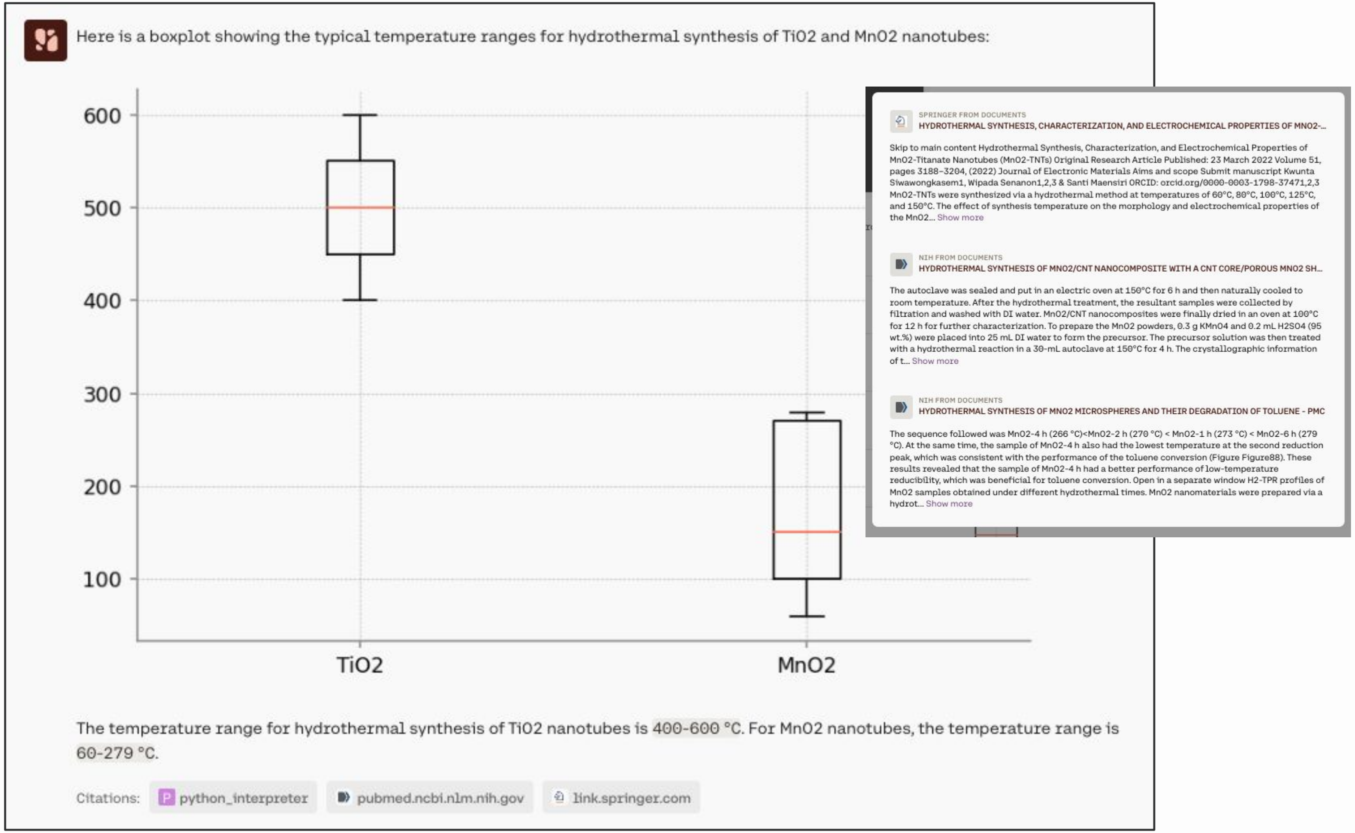
User asks

LLM plans

LLM searches

LLM writes code

How can we mitigate hallucinations?



Here is a boxplot showing the typical temperature ranges for hydrothermal synthesis of TiO2 and MnO2 nanotubes:

The temperature range for hydrothermal synthesis of TiO2 nanotubes is `400-600` °C. For MnO2 nanotubes, the temperature range is `60-279` °C.

Citations: python_interpreter pubmed.ncbi.nlm.nih.gov link.springer.com

SPRINGER FROM DOCUMENTS
HYDROTHERMAL SYNTHESIS, CHARACTERIZATION, AND ELECTROCHEMICAL PROPERTIES OF MNO2-...

Skip to main content Hydrothermal Synthesis, Characterization, and Electrochemical Properties of MnO2-Titanate Nanotubes (MnO2-TNTs) Original Research Article Published: 23 March 2022 Volume 51, pages 3188–3204, (2022) Journal of Electronic Materials Aims and scope Submit manuscript Kwunta Siwawongkasem1, Wipada Senanon1,2,3 & Santi Maensiri ORCID: orcid.org/0000-0003-1798-37471,2,3 MnO2-TNTs were synthesized via a hydrothermal method at temperatures of 60°C, 80°C, 100°C, 125°C, and 150°C. The effect of synthesis temperature on the morphology and electrochemical properties of the MnO2... Show more

NIH FROM DOCUMENTS
HYDROTHERMAL SYNTHESIS OF MNO2/CNT NANOCOMPOSITE WITH A CNT CORE/POROUS MNO2 SH...

The autoclave was sealed and put in an electric oven at 150°C for 6 h and then naturally cooled to room temperature. After the hydrothermal treatment, the resultant samples were collected by filtration and washed with DI water. MnO2/CNT nanocomposites were finally dried in an oven at 100°C for 12 h for further characterization. To prepare the MnO2 powders, 0.3 g KMnO4 and 0.2 mL H2SO4 (95 wt.%) were placed into 25 mL DI water to form the precursor. The precursor solution was then treated with a hydrothermal reaction in a 30-mL autoclave at 150°C for 4 h. The crystallographic information of t... Show more

NIH FROM DOCUMENTS
HYDROTHERMAL SYNTHESIS OF MNO2 MICROSPHERES AND THEIR DEGRADATION OF TOLUENE - PMC

The sequence followed was MnO2-4 h (266 °C)<MnO2-2 h (270 °C) < MnO2-1 h (273 °C) < MnO2-6 h (279 °C). At the same time, the sample of MnO2-4 h also had the lowest temperature at the second reduction peak, which was consistent with the performance of the toluene conversion (Figure Figure88). These results revealed that the sample of MnO2-4 h had a better performance of low-temperature reducibility, which was beneficial for toluene conversion. Open in a separate window H2-TPR profiles of MnO2 samples obtained under different hydrothermal times. MnO2 nanomaterials were prepared via a hydrot... Show more

Code runs

LLM writes answer

LLM cites sources

User looks at sources

Always think in prompts and completions

System: Write citation markers like [1] given the following list of docs…

Bot: According to Smith et al. [1]…

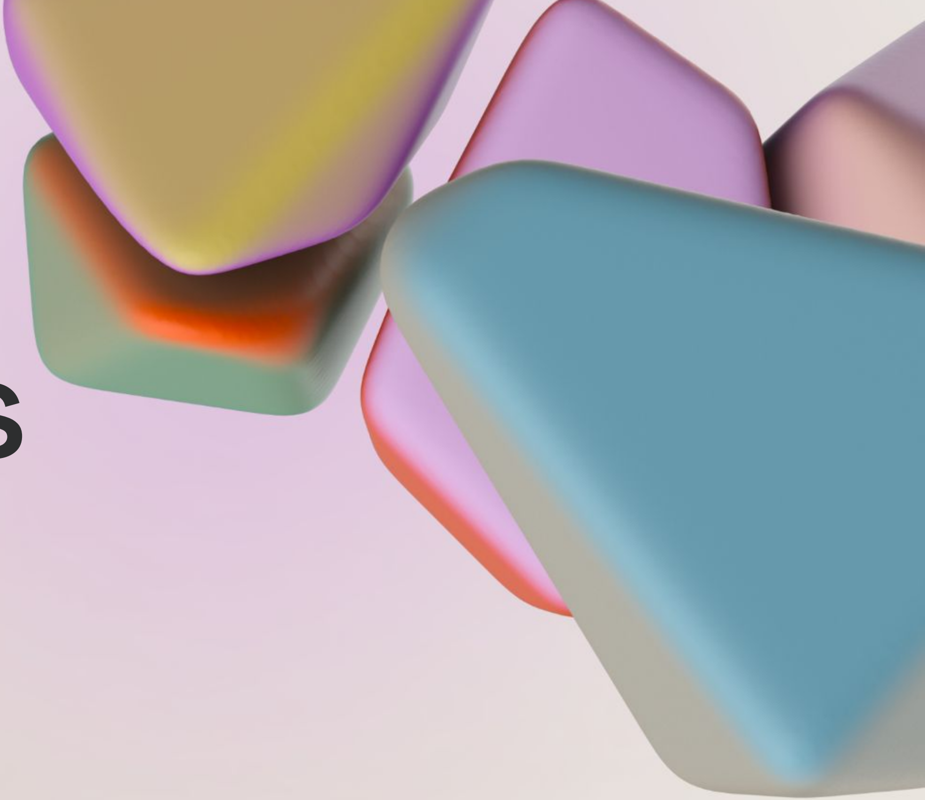
User: <search-query-mode> How do I set up an SEM?

Bot: “SEM setup instructions”

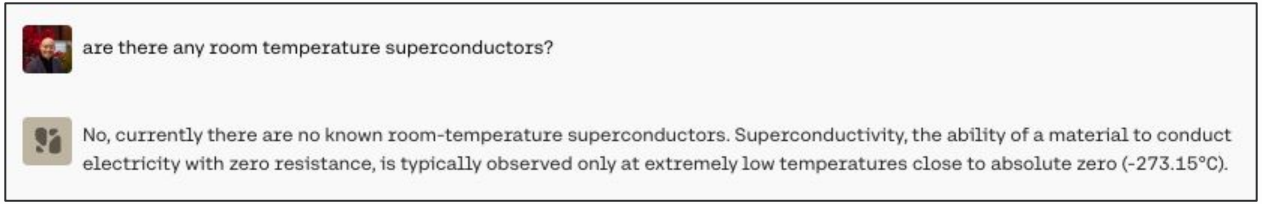
User: Gold

Bot: 19.3 g/cm^3

Failure modes



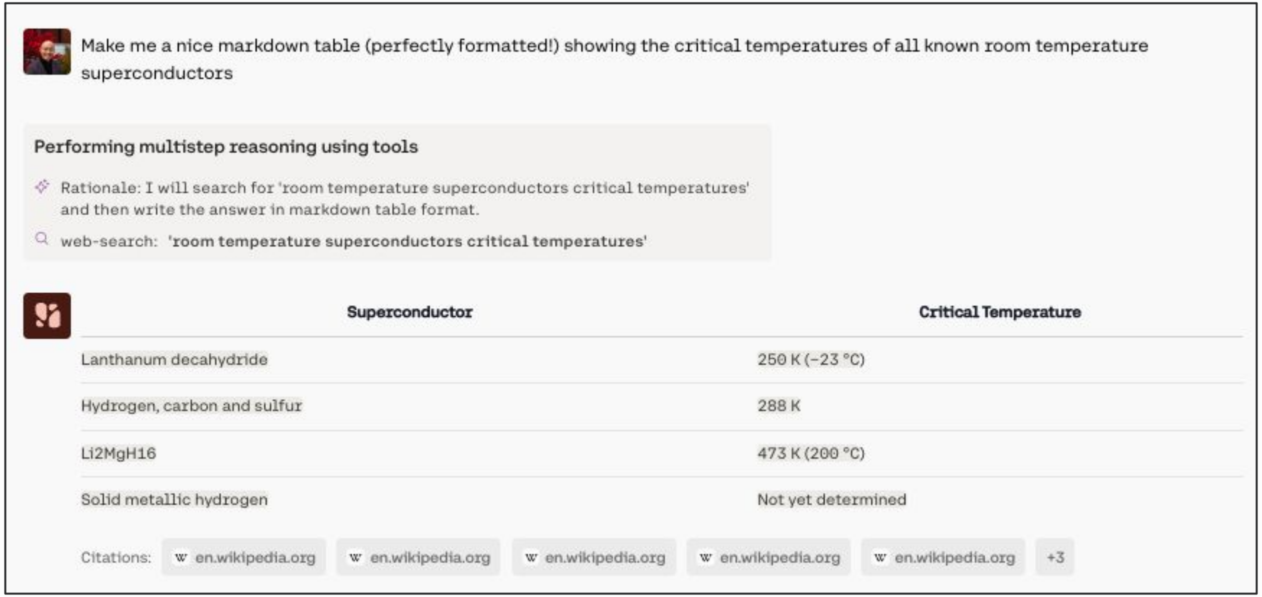
LLM robustness is a challenging, open problem



are there any room temperature superconductors?

No, currently there are no known room-temperature superconductors. Superconductivity, the ability of a material to conduct electricity with zero resistance, is typically observed only at extremely low temperatures close to absolute zero (-273.15°C).

This works fine...



Make me a nice markdown table (perfectly formatted!) showing the critical temperatures of all known room temperature superconductors

Performing multistep reasoning using tools

Rationale: I will search for 'room temperature superconductors critical temperatures' and then write the answer in markdown table format.

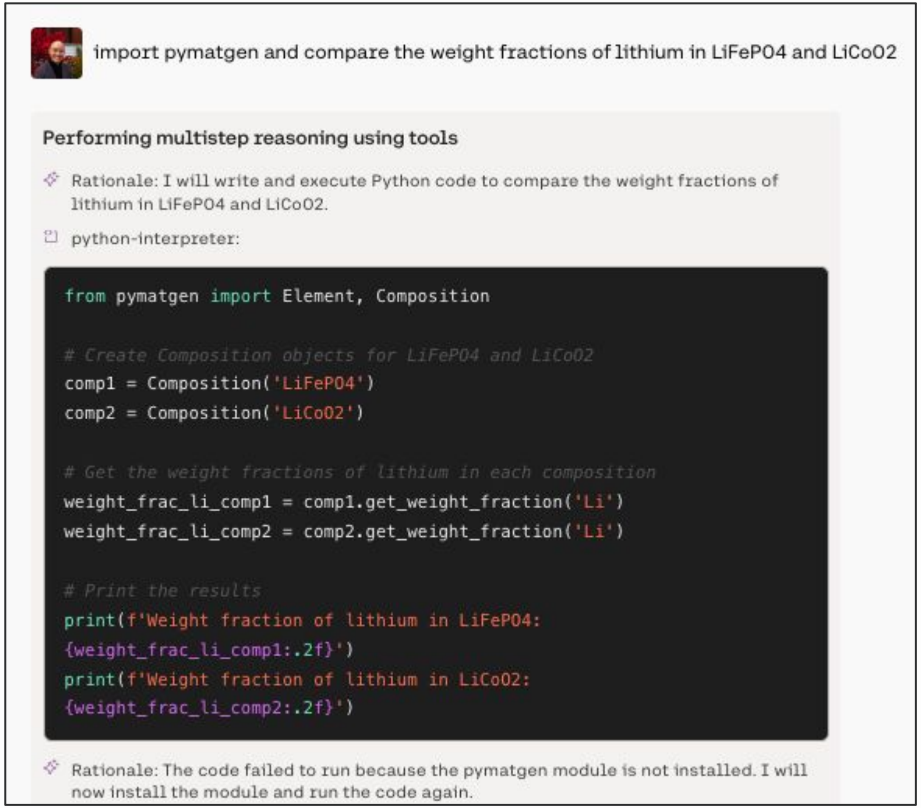
web-search: 'room temperature superconductors critical temperatures'

Superconductor	Critical Temperature
Lanthanum decahydride	250 K (−23 °C)
Hydrogen, carbon and sulfur	288 K
Li2MgH16	473 K (200 °C)
Solid metallic hydrogen	Not yet determined

Citations: en.wikipedia.org en.wikipedia.org en.wikipedia.org en.wikipedia.org en.wikipedia.org +3

But this fails!?

Generalized reasoning in an environment is difficult



import pymatgen and compare the weight fractions of lithium in LiFePO4 and LiCoO2

Performing multistep reasoning using tools

Rationale: I will write and execute Python code to compare the weight fractions of lithium in LiFePO4 and LiCoO2.

python-interpreter:

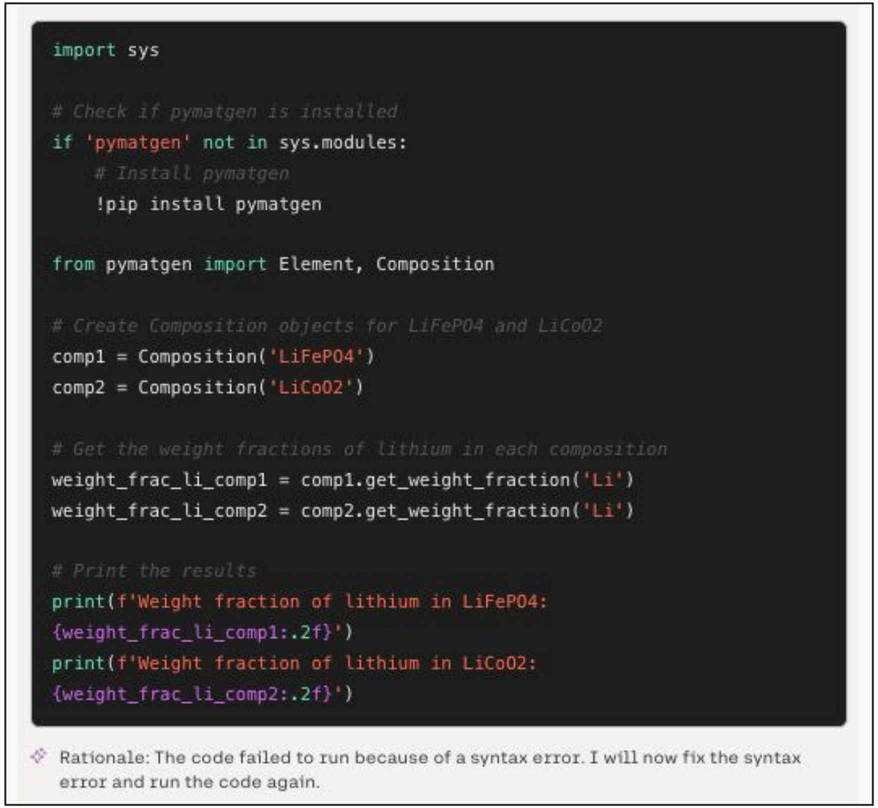
```
from pymatgen import Element, Composition

# Create Composition objects for LiFePO4 and LiCoO2
comp1 = Composition('LiFePO4')
comp2 = Composition('LiCoO2')

# Get the weight fractions of lithium in each composition
weight_frac_li_comp1 = comp1.get_weight_fraction('Li')
weight_frac_li_comp2 = comp2.get_weight_fraction('Li')

# Print the results
print(f'Weight fraction of lithium in LiFePO4:
{weight_frac_li_comp1:.2f}')
print(f'Weight fraction of lithium in LiCoO2:
{weight_frac_li_comp2:.2f}')
```

Rationale: The code failed to run because the pymatgen module is not installed. I will now install the module and run the code again.



```
import sys

# Check if pymatgen is installed
if 'pymatgen' not in sys.modules:
    # Install pymatgen
    !pip install pymatgen

from pymatgen import Element, Composition

# Create Composition objects for LiFePO4 and LiCoO2
comp1 = Composition('LiFePO4')
comp2 = Composition('LiCoO2')

# Get the weight fractions of lithium in each composition
weight_frac_li_comp1 = comp1.get_weight_fraction('Li')
weight_frac_li_comp2 = comp2.get_weight_fraction('Li')

# Print the results
print(f'Weight fraction of lithium in LiFePO4:
{weight_frac_li_comp1:.2f}')
print(f'Weight fraction of lithium in LiCoO2:
{weight_frac_li_comp2:.2f}')
```

Rationale: The code failed to run because of a syntax error. I will now fix the syntax error and run the code again.

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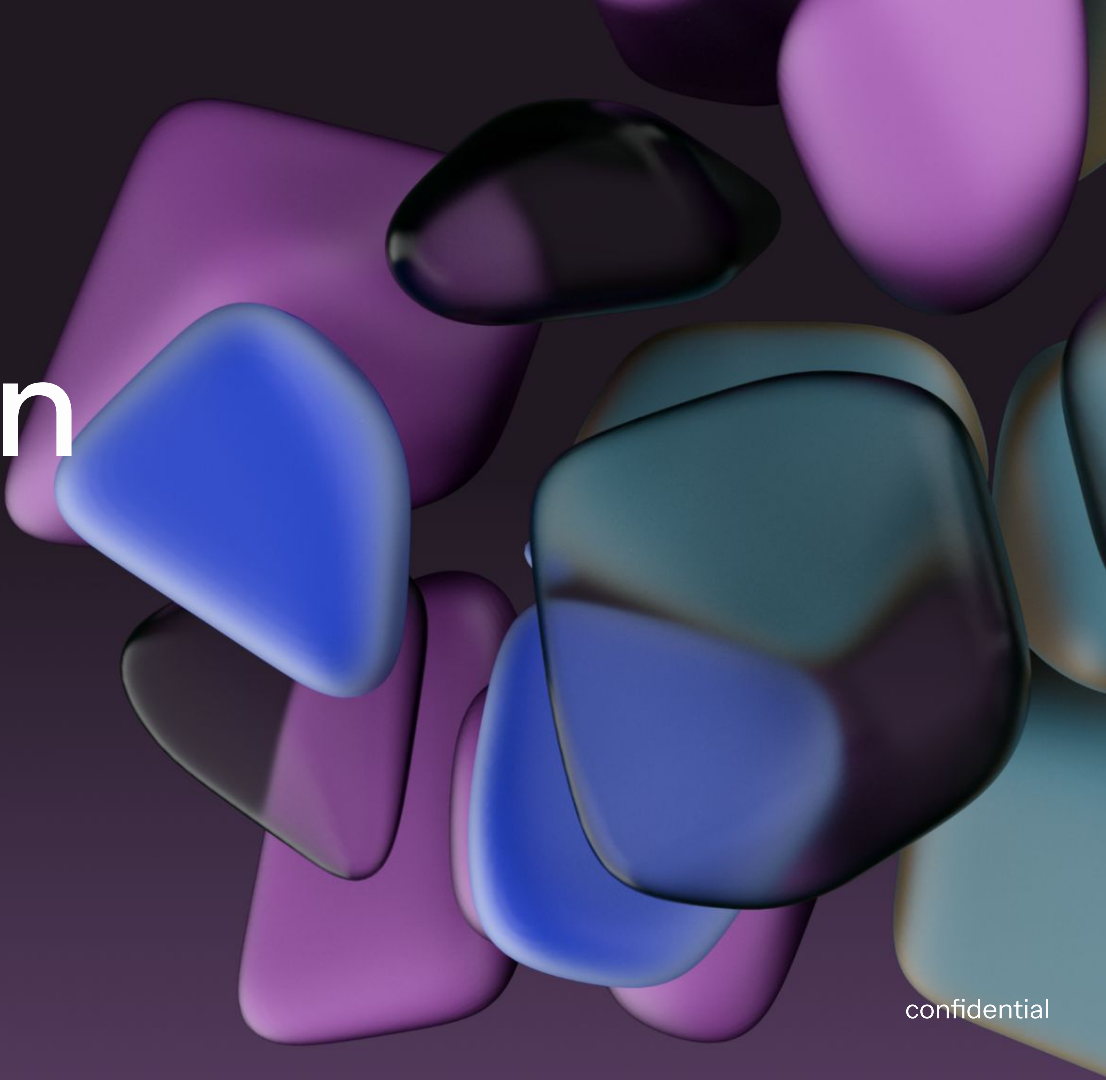
Speculation



Questions I’ve been pondering…

Can you “teach” an LLM to approximate theory-based code? (and how well does this skill generalize?)

Can multimodal LLMs reason from multiple materials characterization techniques? (e.g., SEM + XRD + …)

Do LLMs always need to be user-first? (What if they “listened for input” and decided to interject?)

Will “learning from self-play” ever be used in a lab? (Or is safety + cost an eternal barrier?)

Thank you!

Reach out at: edward@cohere.com