AI FOR ACCELERATED MATERIALS DISCOVERY

CITRINE INFORMATICS

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CEO

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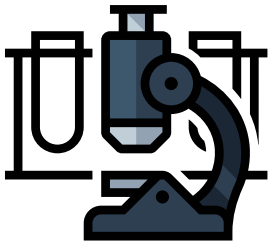
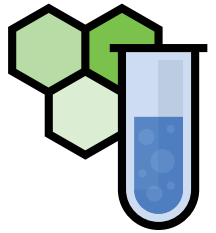
USE SMARTER | USE LESS | USE LONGER

HYPOTHESIZE

TEST



ITERATE



AI-DRIVEN HYPOTHESES: FEWER EXPERIMENTAL CYCLES

OPTIMAL RESULTS

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MATERIALS: A UNIQUE AI USE CASE

	Traditional AI Applications	Materials AI Applications
Datasets	Big, dense (up to ~10^8 examples)	Small, sparse (~10^2 examples)
Prediction task	Pattern-match common cases	Predict unusual or "extreme" chemistries
Hierarchical relationships	Usually not applicable	Inherently hierarchical
Existing Domain Knowledge	No—rely on data to learn patterns	Large body of known materials physics
Outliers	Can be deleted as noise	Often the design goal
Negatives	Not inherently different from positives	Scarce and stigmatized
Data acquisition cost	Data provided by users for free	One data point can cost $millions
Uncertainty in data and models	Usually unimportant	Always important
Interpretability	Usually unimportant	Always important

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LETTER

doi:10.1038/nature23894

3D printing of high-strength aluminium alloys

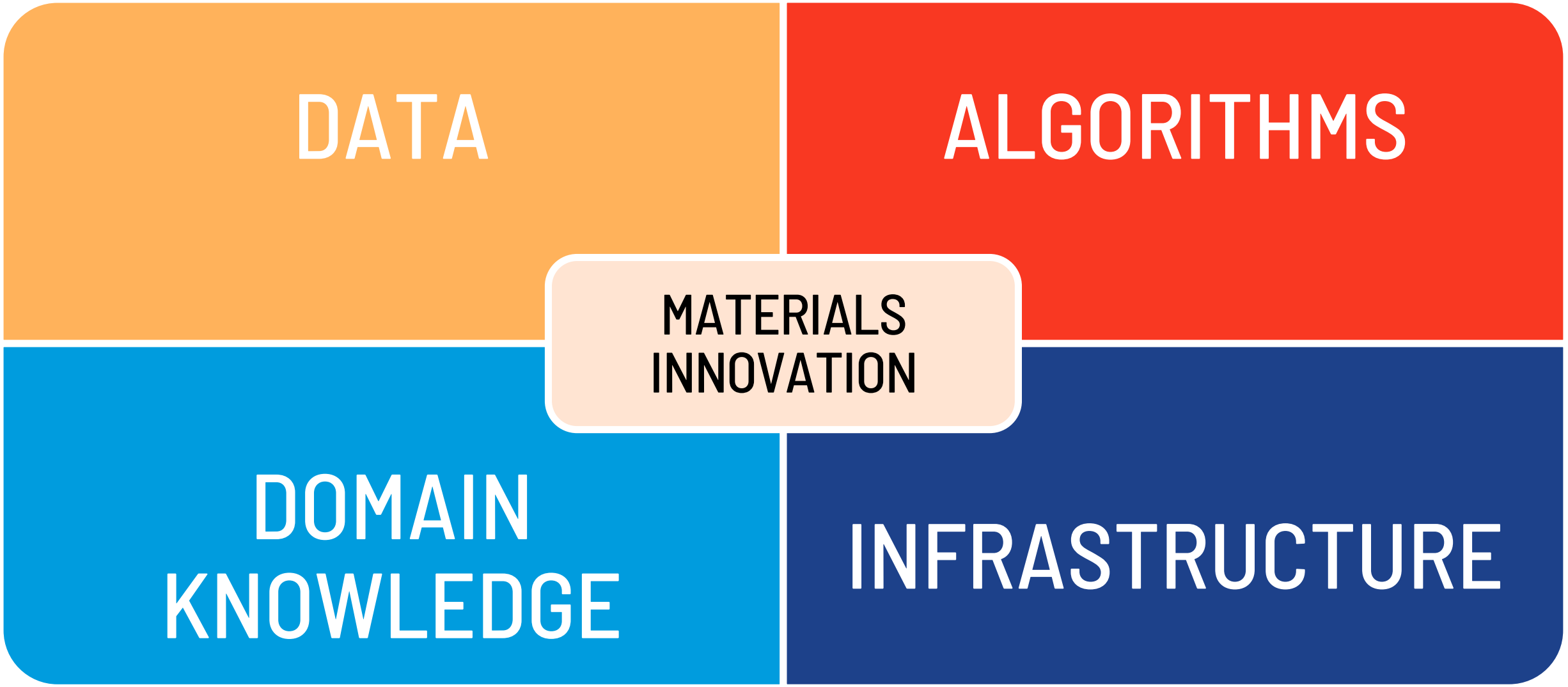
John H. Martin[1,2], Brennan D. Yahata[1], Jacob M. Hundley[1], Justin A. Mayer[1], Tobias A. Schaedler[1] & Tresa M. Pollock[2]

HRL LABORATORIES

UCSB

- Only a few of 5,500 available alloys can be 3D printed; most crack
- Creating new alloys: better decisions

What would've taken years, Citrine narrowed it down to days.
-J.H. Martin, HRL Labs



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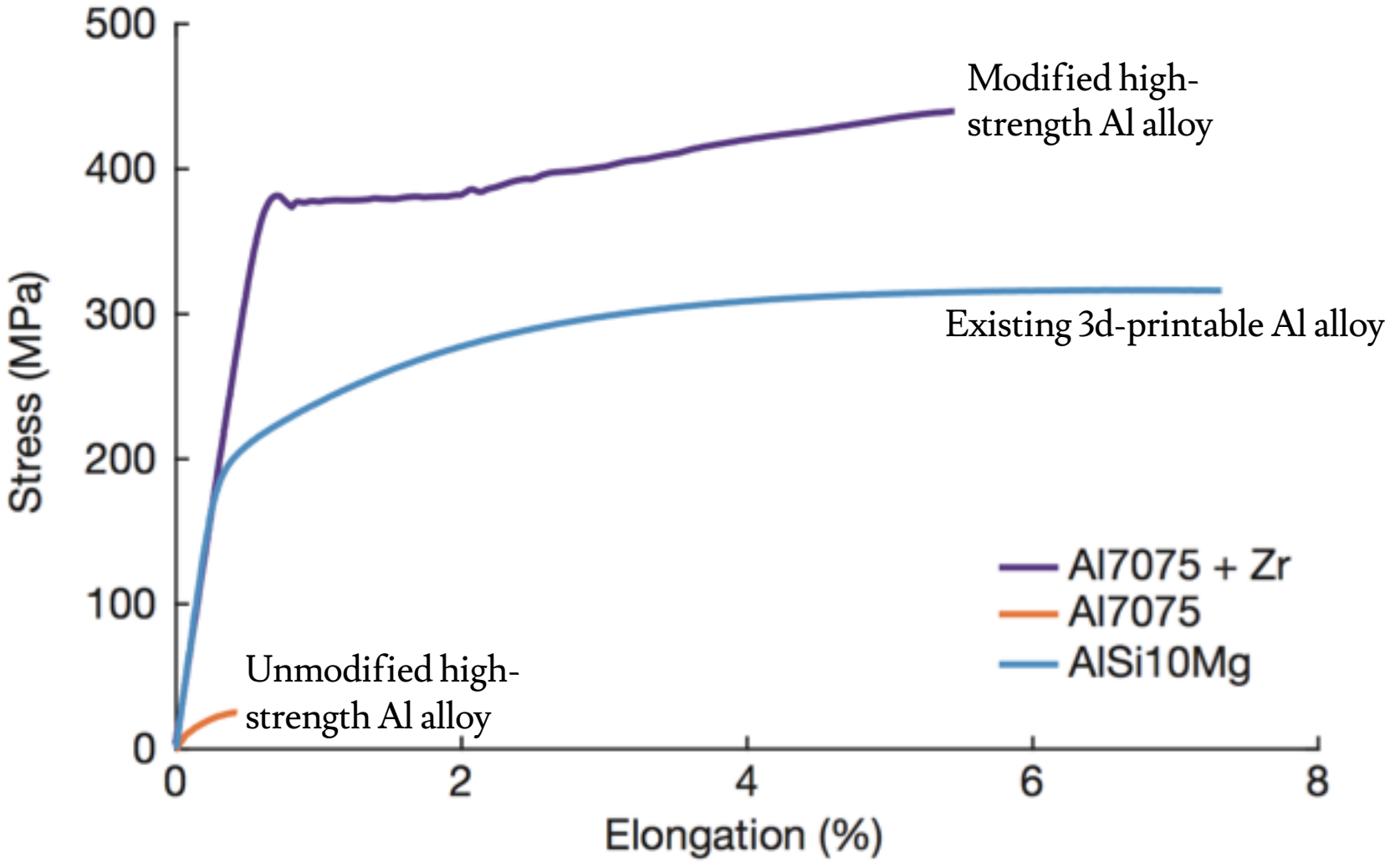
RESULTS



JH Martin et al., *Nature* (2017)

USE LESS

EASIER TO RECYCLE THAN OTHER 3-D PRINTABLE ALLOYS

BUY-TO-FLY RATIO REDUCED BY 50-80%

Saving of metal in a measure of at least 80% is benefited when considering LBW as an alternative to machining – Caiazzo, et. al. (2017)

MORE ADVANCED STRUCTURES AND LESS CRACKING ENABLES LIGHTER WEIGHT

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RECYCLING AND ENVIRONMENTAL IMPACT

Create new recyclable, environmentally friendly options for 3-D printed alloys.

	Material	Recyclability	Earth Abundance	Elemental Toxicity	Conflict Minerals
	$TiAl_6V_4$	Very Low	Medium	Low	No
	Inconel 718	Medium	Low	Medium	Yes
	CoCr	Low	Low	Medium	Yes
This Work	Al 6061	High	High	Low	No
This Work	Al 7075	High	High	Low	No

AI: PROVEN IN MANY MATERIALS DOMAINS

- Batteries (anode, cathode, electrolyte)
- Catalysts
- Formulations
- Phosphors
- Structural Alloys
- Conductive Alloys
- Semiconductors
- Glasses
- Optical emitters
- Thermoelectrics
- Solid state ion conductors
- Solar absorbers
- Thermosets
- Thermoplastics
- And many more...

AI+MATERIALS: INGREDIENTS FOR SUCCESS

- AI is really about data, not magic algorithms
- AI should be designed for materials applications
  - Focus specifically on small, sparse data
  - Respect and leverage laws of physics
- We need sophisticated infrastructure to store, inspect, and share data
- AI isn't a switch-flip; it requires culture and process changes
- Replacing experiment is a pipe dream, but greatly reducing experimental burden is here today
- AI cannot be a black box—scientists will not trust it
- Training in AI for scientists—need to be "bilingual"

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