

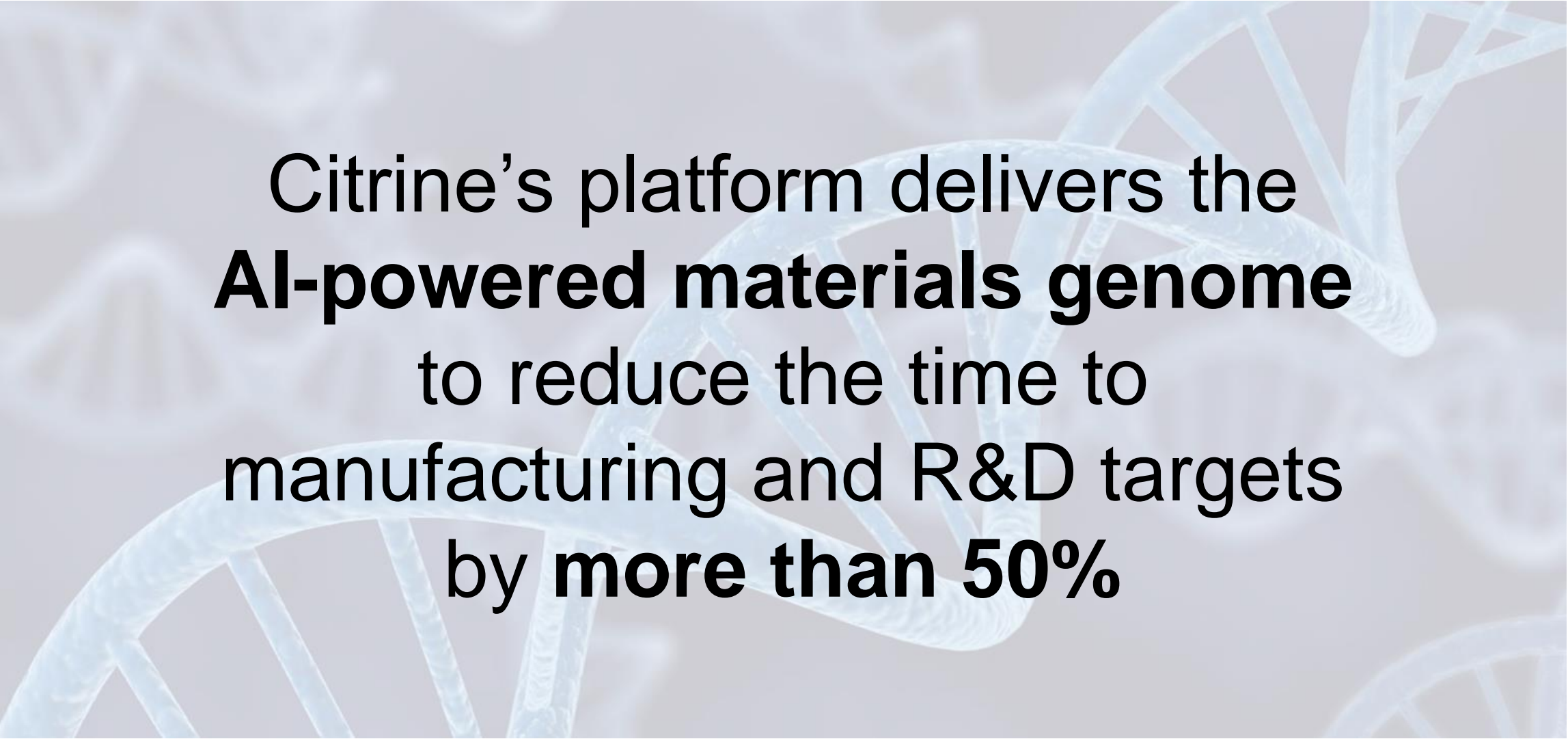


Citrine Informatics

The data analytics platform for the physical world

Materials Informatics: Artificial Intelligence Driven Materials Development and Optimization

November 29, 2016




Citrine's platform delivers the
AI-powered materials genome
to reduce the time to
manufacturing and R&D targets
by **more than 50%**

Citrine's Questions

“How do we identify promising new materials quickly?”

“How do we optimize known materials systems to achieve target results?”

“How do we fill in unknown information about known materials?”

 Search Predict

General

SHOW FILTERS TOGGLE COLUMNS ENABLE ALL DISABLE ALL

	General	Processing	Properties	
Record	Chemical formula	Temper	Elongation	Brinell hardness
View	Al _{95.28} Cr _{0.19} Fe _{0.41} Mg _{2.68} Mn _{0.81} Si _{0.21} Ti _{0.18} Zn _{0.24}	H34	13 %	81
View	Al _{81.39} Cu _{3.51} Fe _{1.93} Mg _{0.08} Mn _{0.57} Ni _{0.41} Si _{8.53} Sn _{0.41} W _{3.17}	F	3 %	80
View	Al _{92.66} Cu _{0.68} Fe _{0.2} Mg _{1.66} Si _{0.1} Zn _{4.7}	T5	15 %	115
View	Al _{90.98} Cu _{0.23} Fe _{0.61} Mg _{0.36} Mn _{0.4} Si _{7.0} Ti _{0.18} Zn _{0.24}	F	5 %	61
View	Al _{99.38} Fe _{0.41} Si _{0.21}	H18	4 %	35
View	Al _{92.85} Cr _{0.19} Fe _{0.4} Mg _{1.4} Mn _{0.4} Si _{0.3} Zn _{4.47}	T53	15 %	105
View	Al _{94.64} Cr _{0.19} Cu _{0.23} Fe _{0.41} Mg _{3.49} Mn _{0.41} Si _{0.21} Ti _{0.18} Zn _{0.24}	H19	5 %	96
View	Al _{89.26} Cu _{4.04} Fe _{1.18} Mg _{0.09} Mn _{0.58} Ni _{0.41} Si _{2.97} Ti _{0.17} W _{1.3}	F	2 %	55
View	Al _{91.49} Cr _{0.19} Cu _{1.16} Fe _{0.61} Mg _{0.53} Mn _{0.6} Si _{5.01} Ti _{0.17} Zn _{0.24}	F	4 %	69
View	Al _{88.22} Cu _{1.86} Fe _{0.2} Mg _{0.53} Si _{9.02} Ti _{0.17}	T62	3 %	105

Showing 1 to 10 of 481 entries

1 2 3 4 5 ... 49



Citrine's Questions [under constraint]

“How do we identify promising new materials quickly?”

“How do we optimize known materials systems to achieve target results?”

“How do we fill in unknown information about known materials?”

[without critical materials]

[only using environmentally sustainable processing]

[with minimal risk to existing product lines]

The Citrine Platform Solution



Shinier Paint



Stronger Steel



Lighter Vehicles




Greener Suppliers




Artificial Intelligence-Based Design Tools
Citrine delivers powerful AI for manufacturers



World's Largest Materials Data Platform
Citrine is consolidating the world's physical knowledge



Data Extraction from Documents
Citrine's extraction engine ingests quantitative data from research papers, patents, data sheets



Data Streaming from Users
Customers and a growing network of government and university labs push data to our platform

Artificial Intelligence

Machine Learning

Cognitive Computing

Artificial Intelligence: Mapping $x_1 \dots x_n$ to y

Goal: Construct a (highly complex and nonlinear) mapping from these x variables (chemistry and processing we can control)...

...to our target y property, fatigue strength

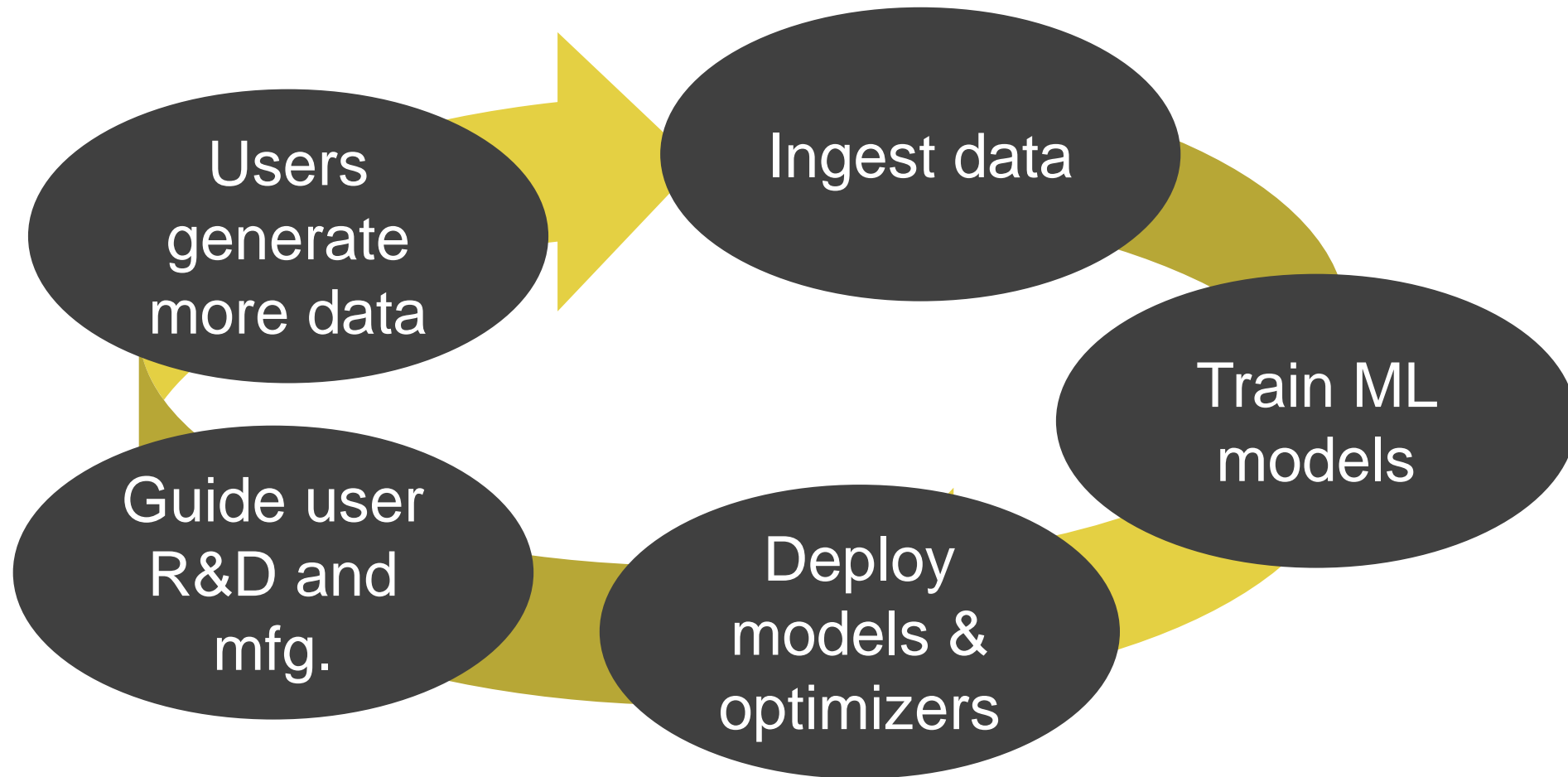
Table 1 NIMS data features

Abbreviation	Details
C	% Carbon
Si	% Silicon
Mn	% Manganese
P	% Phosphorus
S	% Sulphur
Ni	% Nickel
Cr	% Chromium
Cu	% Copper
Mo	% Molybdenum
NT	Normalizing Temperature
THt	Through Hardening Temperature
THt	Through Hardening Time
THQCr	Cooling Rate for Through Hardening
CT	Carburization Temperature
Ct	Carburization Time
DT	Diffusion Temperature
Dt	Diffusion time
QmT	Quenching Media Temperature (for Carburization)
TT	Tempering Temperature
Tt	Tempering Time
TCr	Cooling Rate for Tempering
RedRatio	Reduction Ratio (Ingot to Bar)
dA	Area Proportion of Inclusions Deformed by Plastic Work
dB	Area Proportion of Inclusions Occurring in Discontinuous Array
dC	Area Proportion of Isolated Inclusions
Fatigue	Rotating Bending Fatigue Strength (10⁷ Cycles)

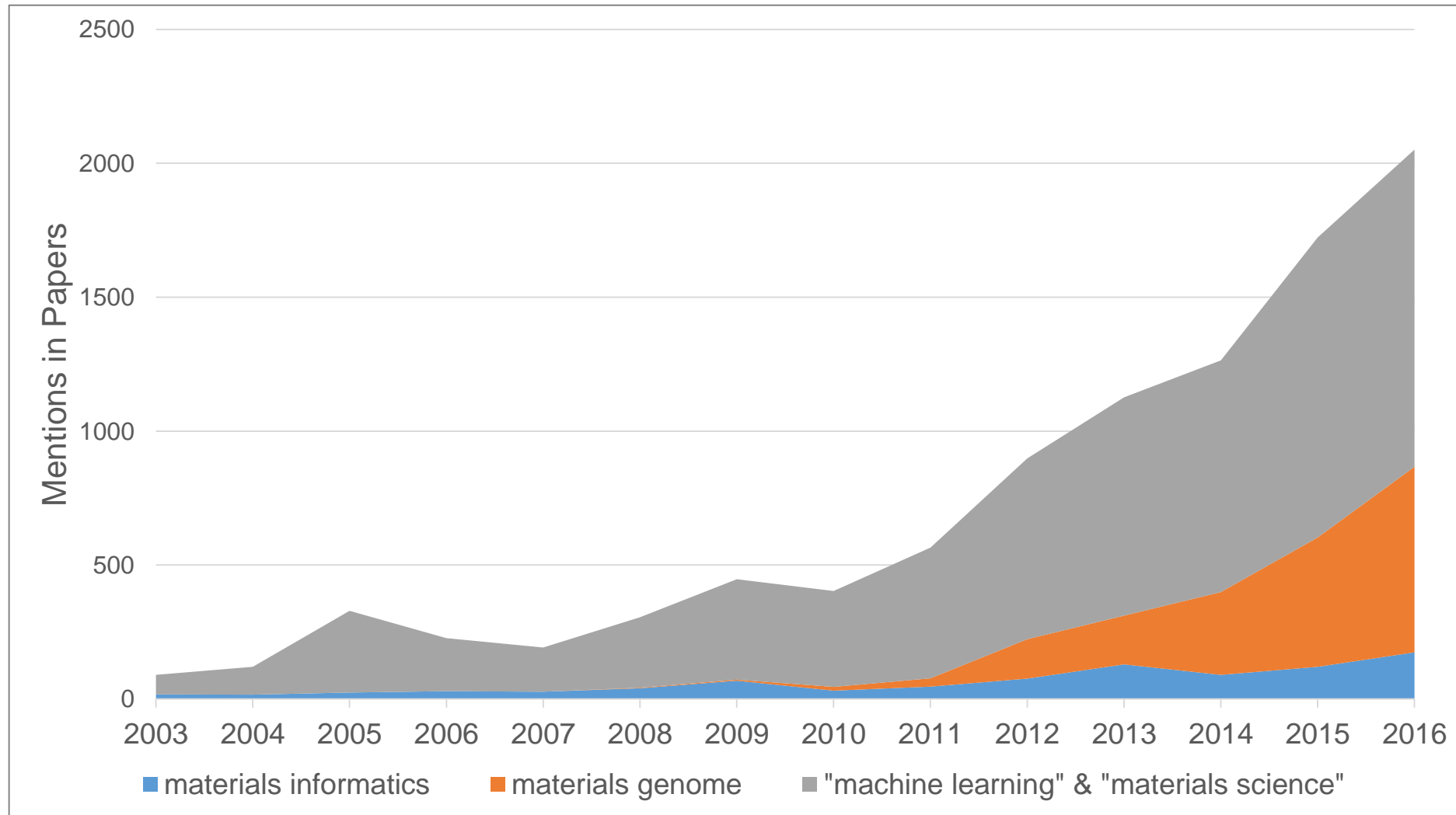


Fatigue Strength

Platform Overview—Virtuous Cycle



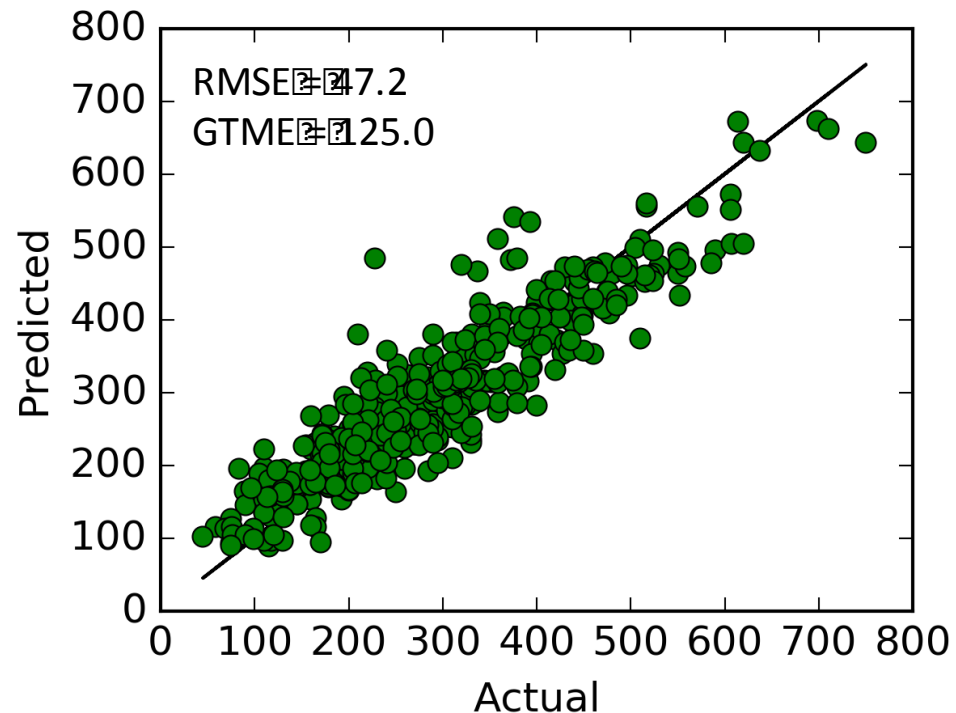
Materials Informatics is growing



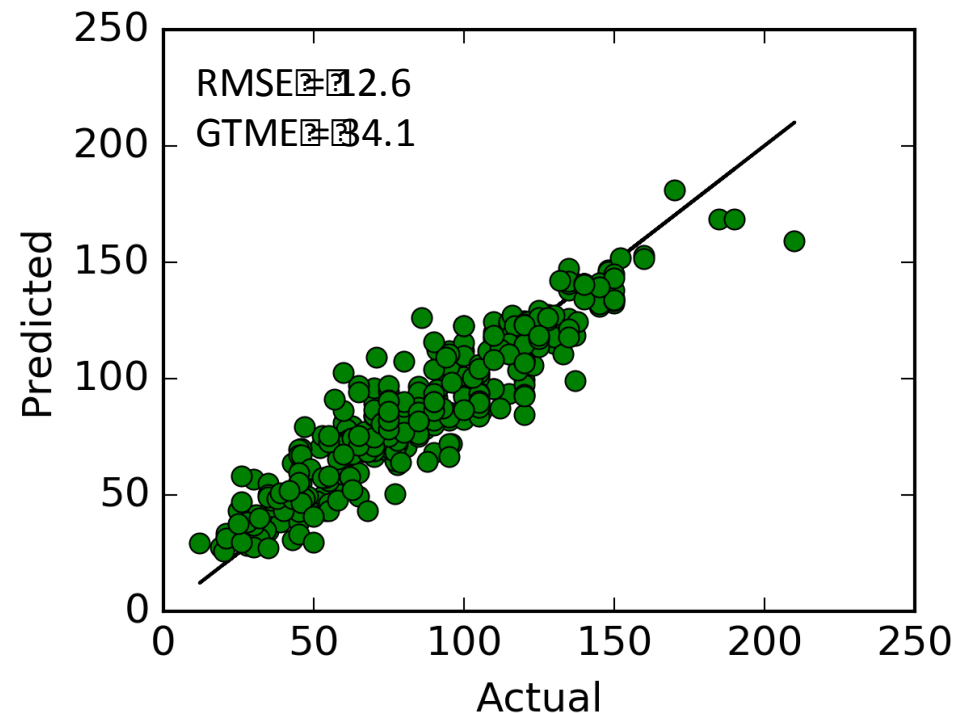
Broad Applications: Aluminum Alloys

Citrine customer goal: lightweight Al-based alloys

Tensile Strength

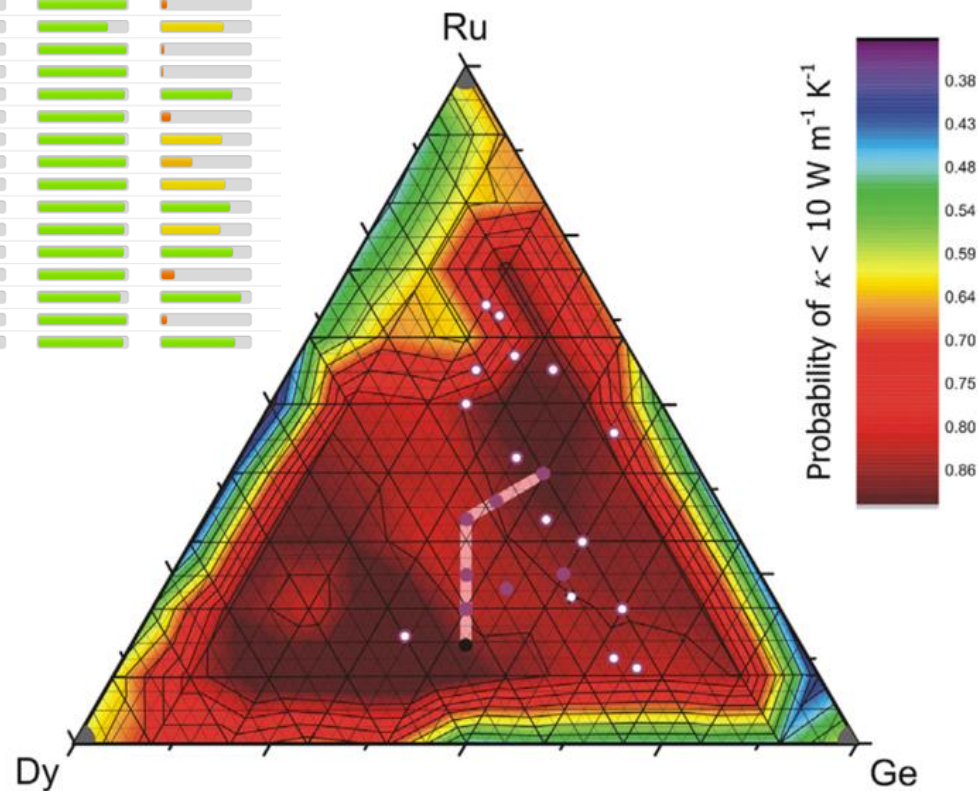


Hardness



Mapping Materials Performance

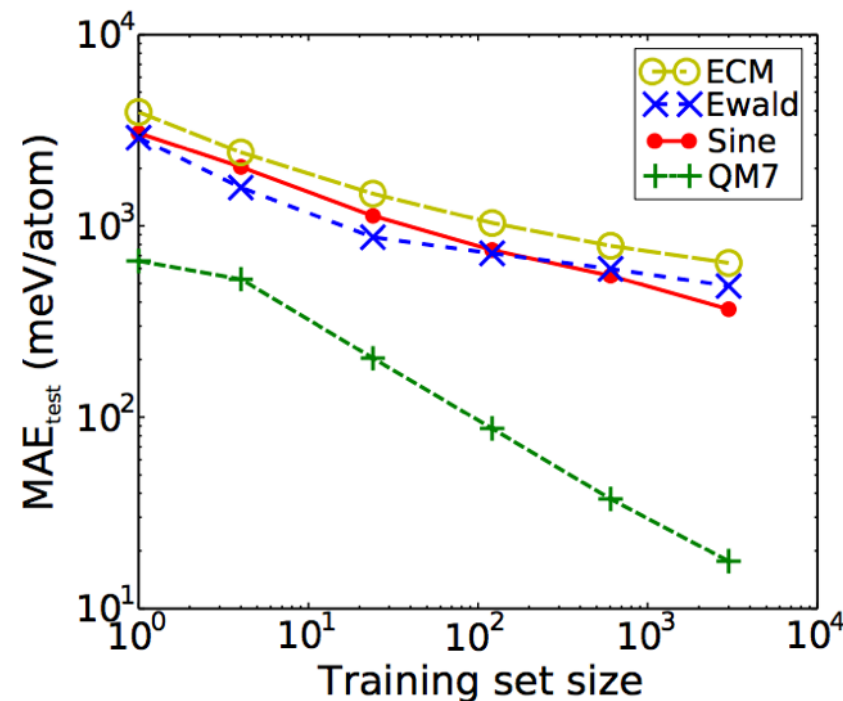
COMPOUND NAME	COMPOUND	SEEBECK COEFFICIENT	RESISTIVITY	THERMAL CONDUCTIVITY	BAND GAP
<input type="text"/>	NbCoSn	<div><div></div></div>	<div><div></div></div>	<div><div></div></div>	<div><div></div></div>
<input type="button" value="SUBMIT"/>	FeAgS ₂	<div><div></div></div>	<div><div></div></div>	<div><div></div></div>	<div><div></div></div>
	InCuPt ₂	<div><div></div></div>	<div><div></div></div>	<div><div></div></div>	<div><div></div></div>
	FeSnRu ₂	<div><div></div></div>	<div><div></div></div>	<div><div></div></div>	<div><div></div></div>
CUTOFFS	MnAlRh ₂	<div><div></div></div>	<div><div></div></div>	<div><div></div></div>	<div><div></div></div>
Seebeck Coefficient	MnZnS ₂	<div><div></div></div>	<div><div></div></div>	<div><div></div></div>	<div><div></div></div>
<div><div></div>0.27</div>	TiNiSn	<div><div></div></div>	<div><div></div></div>	<div><div></div></div>	<div><div></div></div>
Resistivity	MnZnSe ₂	<div><div></div></div>	<div><div></div></div>	<div><div></div></div>	<div><div></div></div>
<div><div></div>0.27</div>	CdFeS ₂	<div><div></div></div>	<div><div></div></div>	<div><div></div></div>	<div><div></div></div>
Thermal Conductivity	InCuS ₂	<div><div></div></div>	<div><div></div></div>	<div><div></div></div>	<div><div></div></div>
<div><div></div>0.27</div>	CuPSe ₂	<div><div></div></div>	<div><div></div></div>	<div><div></div></div>	<div><div></div></div>
Band Gap	AlCuSe ₂	<div><div></div></div>	<div><div></div></div>	<div><div></div></div>	<div><div></div></div>
<div><div></div>0.27</div>	VFeSb	<div><div></div></div>	<div><div></div></div>	<div><div></div></div>	<div><div></div></div>
	BiPd ₂ Pb	<div><div></div></div>	<div><div></div></div>	<div><div></div></div>	<div><div></div></div>
	TaCuO ₃	<div><div></div></div>	<div><div></div></div>	<div><div></div></div>	<div><div></div></div>
Citrine Informatics	FeAgTe ₂	<div><div></div></div>	<div><div></div></div>	<div><div></div></div>	<div><div></div></div>
Contact About	TiCoSb	<div><div></div></div>	<div><div></div></div>	<div><div></div></div>	<div><div></div></div>
Copyright 2014					



Our platform predicts materials properties by looking for patterns in how other materials behave

Model Quality vs. Training Database Size

Note: this is a log scale!
Large quantities of training data are very important!



Faber, F., Lindmaa, A., von Lilienfeld, O. A., & Armiento, R. (2015). Crystal structure representations for machine learning models of formation energies. *International Journal of Quantum Chemistry*, 115(16), 1094-1101.

Incentives

Publishers Survive and thrive in new world of open data

Institutions Share key findings, continue to next development

Companies Get to market faster, preserve lead

Self-Sustaining Successes

Funded by top-tier Silicon Valley venture capitalists

Partnerships with national labs and universities

Work with Forbes Global 1000 companies



Citrine Informatics

The data analytics platform for the physical world

Thank you

greg@citrine.io

<http://www.citrine.io>

Learn More at Citrine.io

The banner features a background of a complex, interconnected molecular or network structure in light gray and yellow. At the top left is the Citrine Informatics logo, consisting of a yellow semi-circle with three internal lines. To its right is the text "Citrine Informatics" in a dark gray sans-serif font. Below the logo and text, the main headline "AI-POWERED MATERIALS INFORMATICS" is written in large, bold, black, all-caps sans-serif font, followed by "ACCELERATING THE GLOBAL 1000" in a slightly smaller, bold, black, all-caps sans-serif font. Underneath the headline, a paragraph of text in a smaller, dark gray sans-serif font reads: "Citrine's machine learning-based platform mines vast quantities of data about materials, chemicals, and processes to help you hit R&D and manufacturing targets in half the time." At the bottom left, there is a black rectangular button with the text "SEE A DEMO" in white, all-caps sans-serif font. To the right of the button, a horizontal navigation menu in a small, dark gray sans-serif font includes the links: "HOME", "NEWS", "PARTNERS", "PAPERS", and "PUBLIC DATA".

 Citrine Informatics

AI-POWERED MATERIALS INFORMATICS ACCELERATING THE GLOBAL 1000

Citrine's machine learning-based platform mines vast quantities of data about materials, chemicals, and processes to help you hit R&D and manufacturing targets in half the time.

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- Read our publications and news
- See some of our current customers & partners