Ref. Ares(2017)13347 - 03/01/2017

Citrine Informatics

The data analytics platform for the physical world

Materials Informatics: Artificial Intelligence Driven Materials Development and Optimization

November 29, 2016

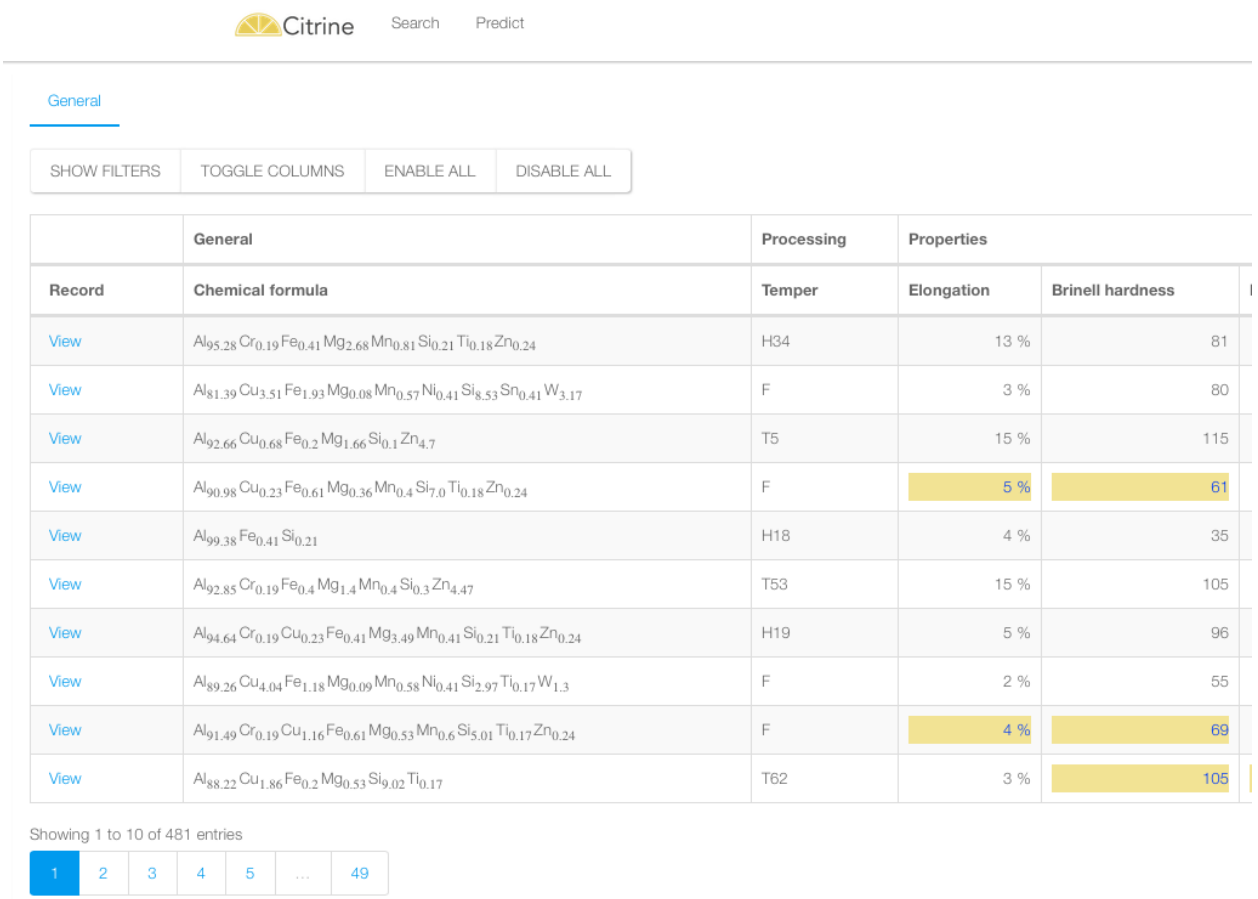
Citrine's platform delivers the **AI-powered materials genome** to reduce the time to manufacturing and R&D targets by **more than 50%**

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?



	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

Confidential and Proprietary

Machine Learning

Confidential and Proprietary

Cognitive Computing

Confidential and Proprietary

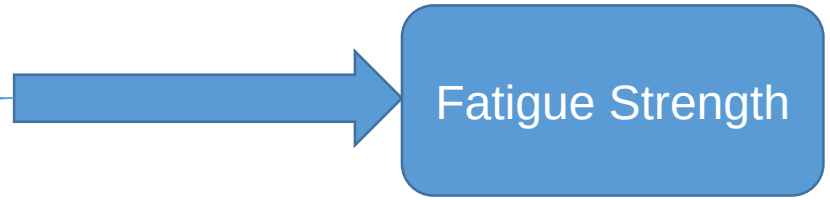
Artificial Intelligence: Mapping $x_1 \ldots x_n$ to y

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

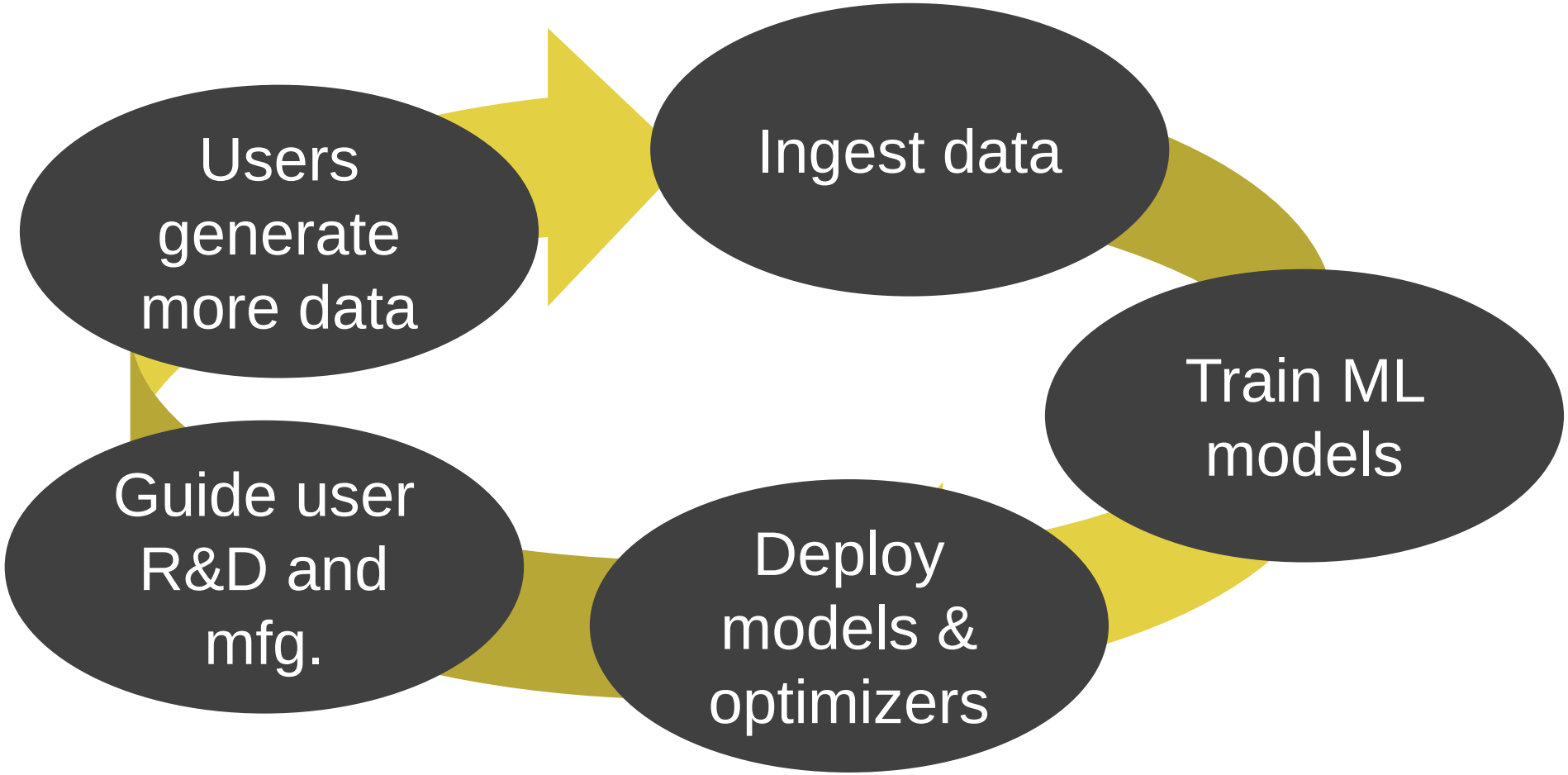
Table 1 NIMS data features

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 (10^7 Cycles)**

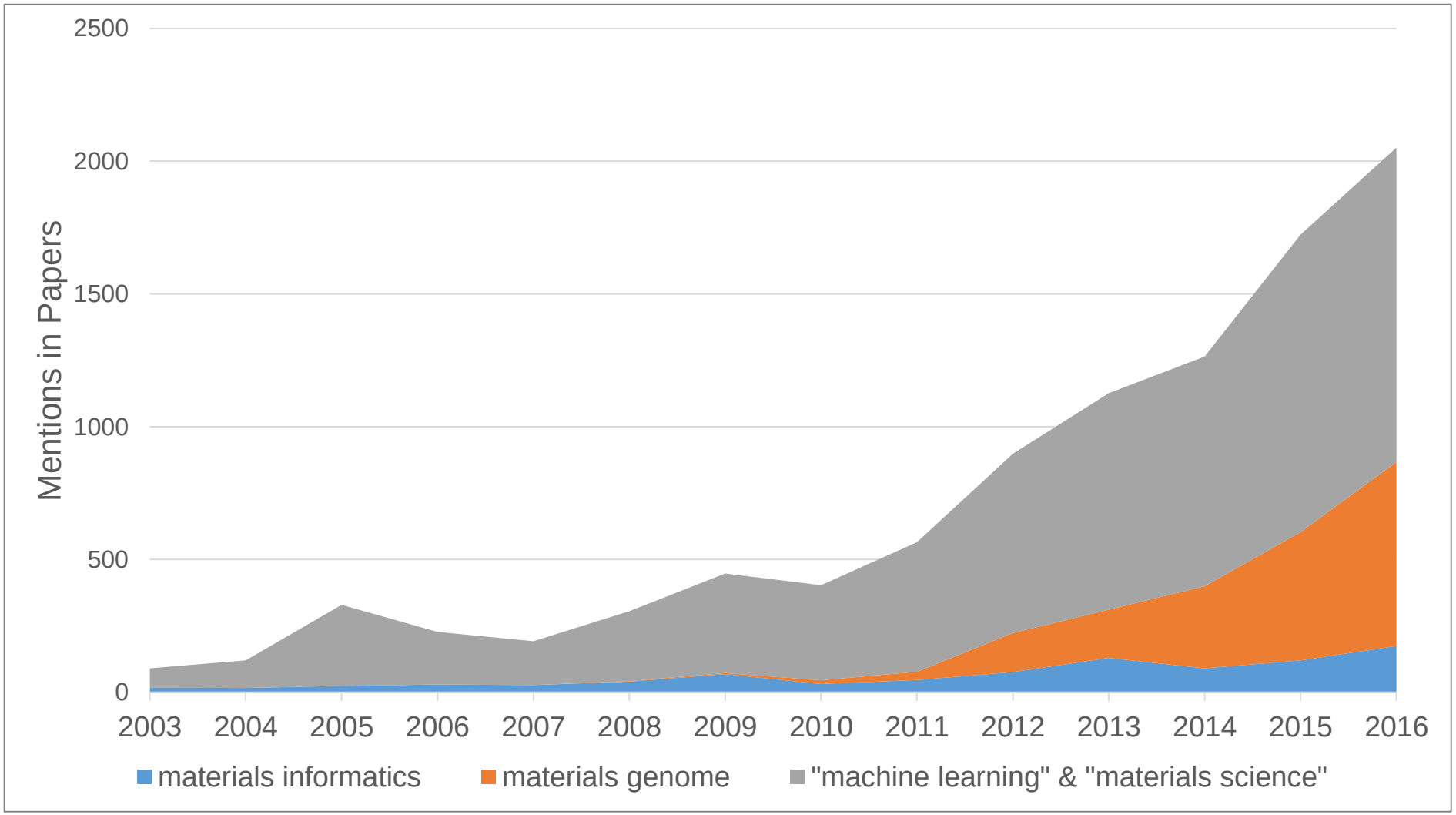


Confidential and Proprietary

Platform Overview—Virtuous Cycle



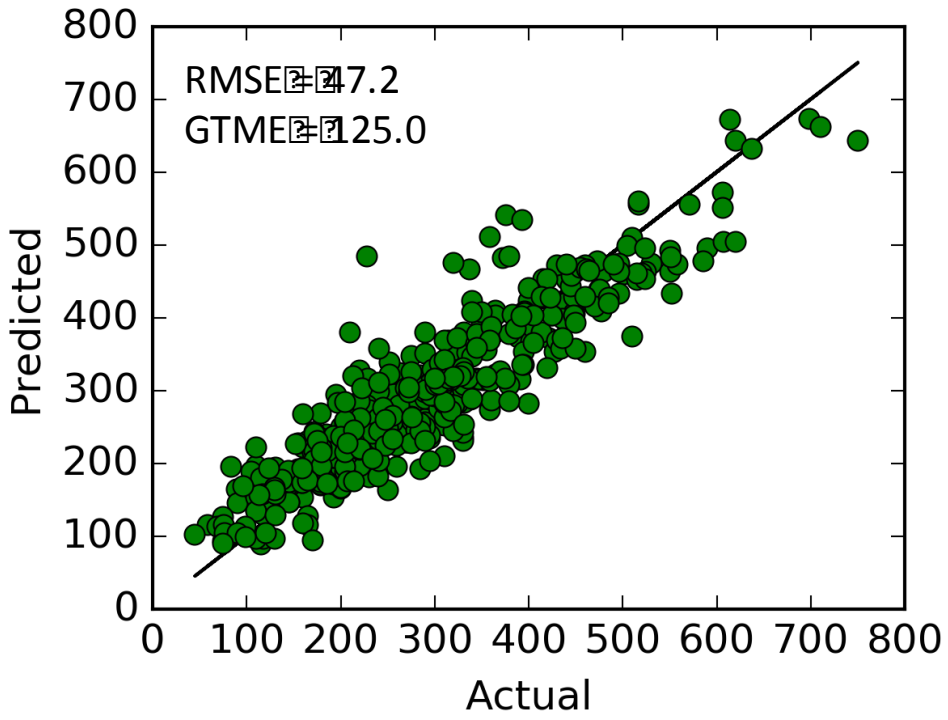
Materials Informatics is growing



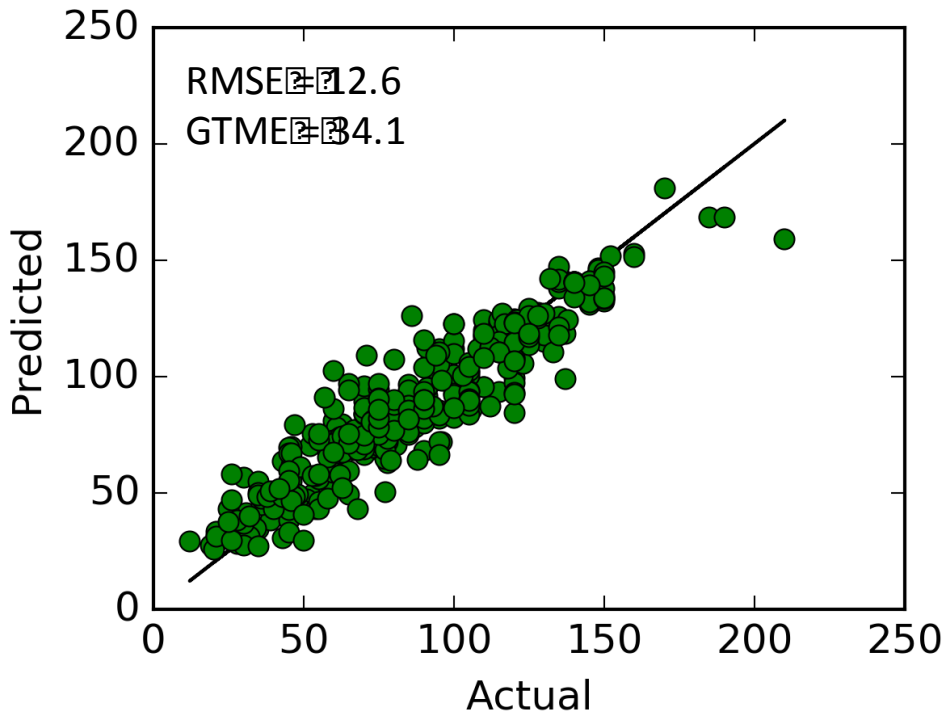
Broad Applications: Aluminum Alloys

Citrine customer goal: lightweight Al-based alloys

Tensile Strength

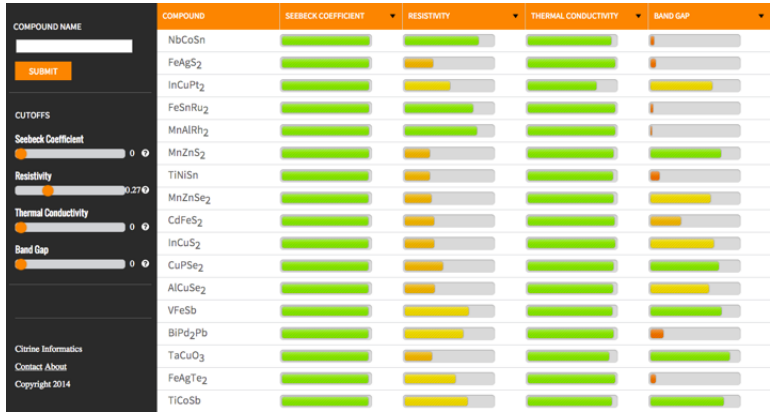


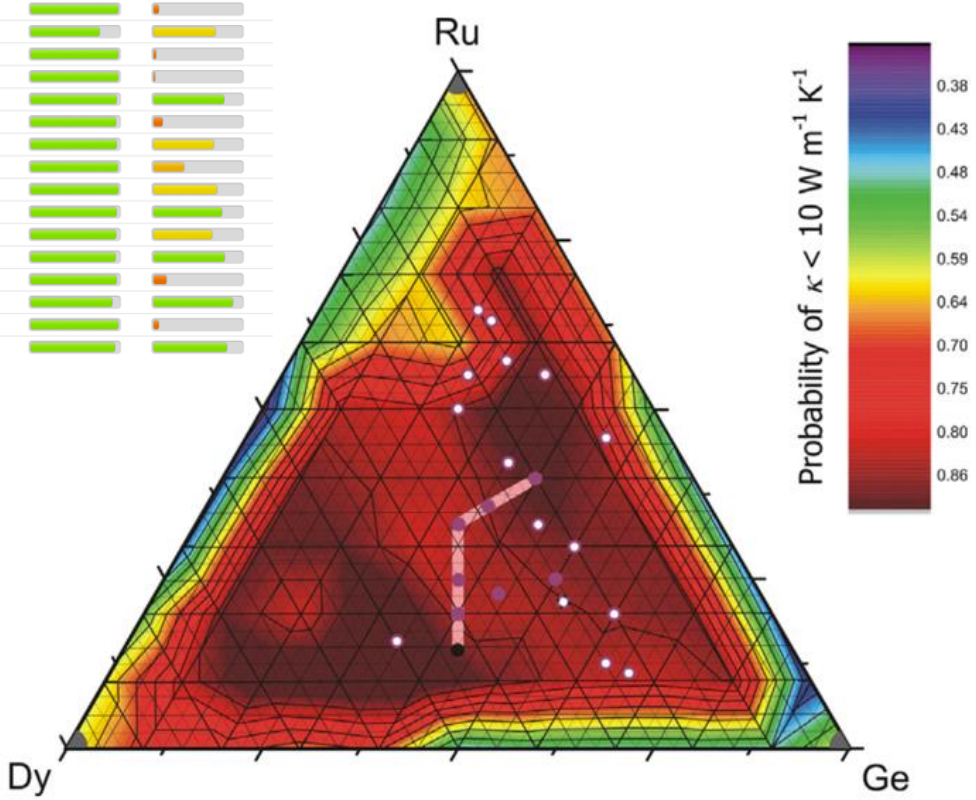
Hardness



For internal use by Citrine customers only

Mapping Materials Performance



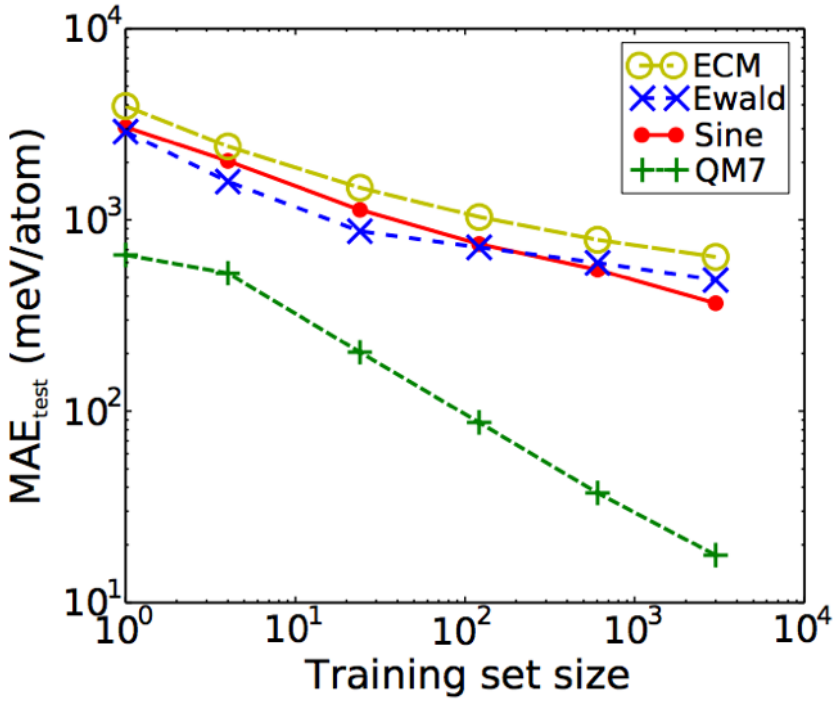


Our platform predicts materials properties by looking for patterns in how other materials behave

Confidential and Proprietary

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.

Confidential and Proprietary

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

- Request a demo
- Meet our world-expert team
- Read our publications and news
- See some of our current customers & partners