Citrine Informatics

The data analytics platform for the physical world

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Lead Architect of Machine Learning

Citrination: Machine Learning for Materials Informatics

You are now defined by

How fast you can move

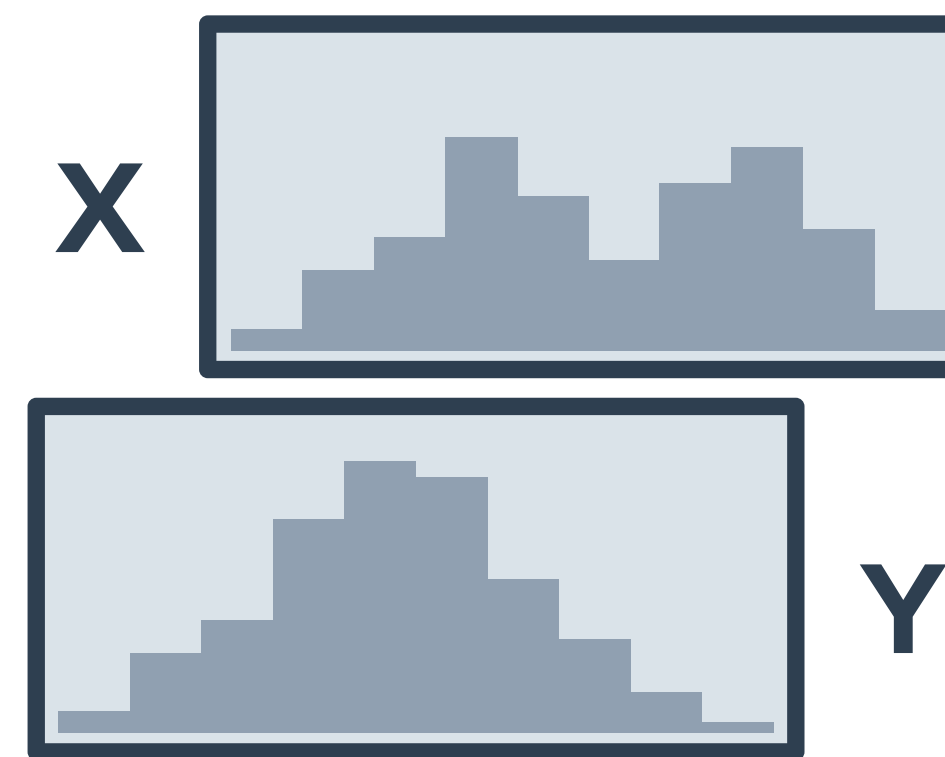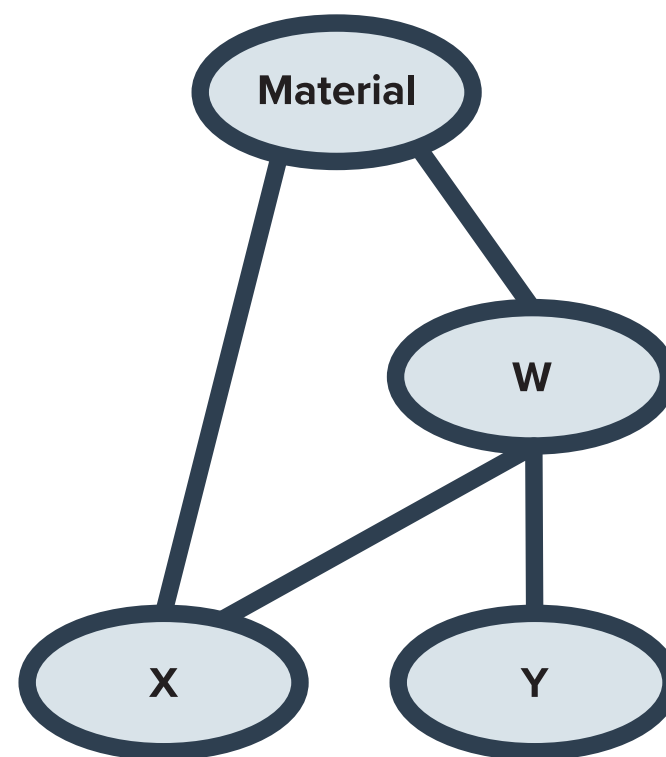# Materials: Analog in a Digital World

- World's reference data is stuck in old books, many formats

- Unstructured and scattered

- Citrination has 2.7 million public records

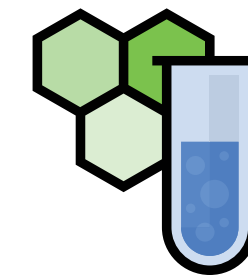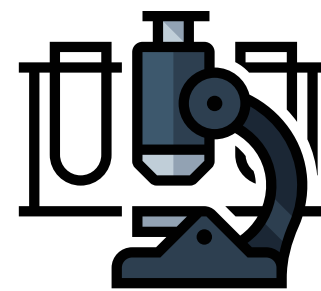# The future of the boundary between AI and materials

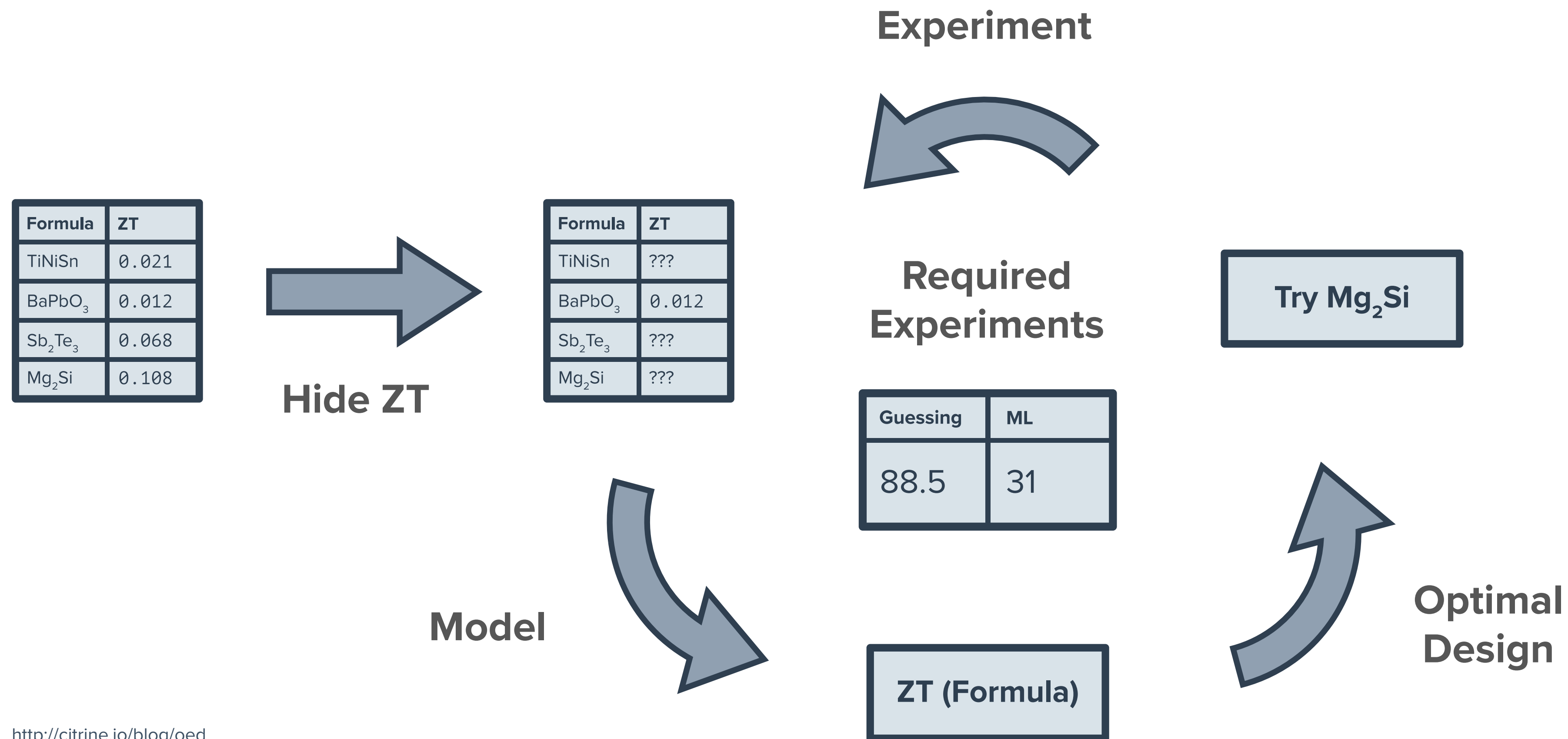Modeling Materials Discovery

Hypothesize → **Test** → **Iterate**

- Intuition driven
- Intuition + data is far more powerful than intuition alone
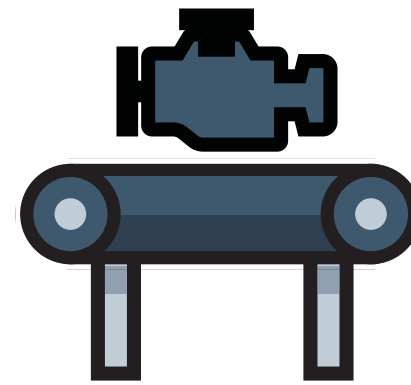- Discovery 2x faster

Search For Thermoelectrics

Formula	ZT
TiNiSn	0.021
$BaPbO_3$	0.012
Sb_2Te_3	0.068
Mg_2Si	0.108

Hide ZT

Formula	ZT
TiNiSn	???
$BaPbO_3$	0.012
Sb_2Te_3	???
Mg_2Si	???

Experiment

Required Experiments

Guessing	ML
88.5	31

Try Mg_2Si

Model

ZT (Formula)

Optimal Design

http://citrine.io/blog/oed
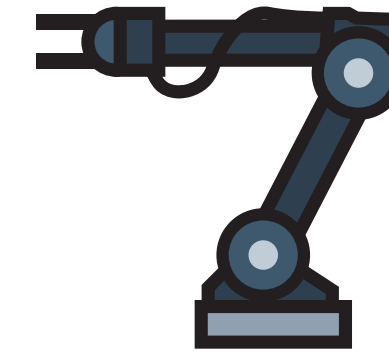
Huge Opportunity

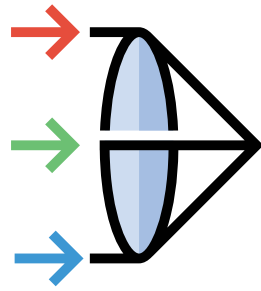Get to Market Faster

Manual → Tools → Automatic

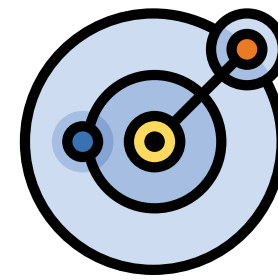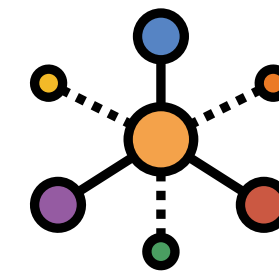Automatization has compounding returns

Products

Ingestion Engine

———

Takes these diverse formats of materials data and brings them into a usable structure

Data Infrastructure

———

Store and host the data in a system that understanding the complexities and subtleties of materials and chemicals data

Artificial Intelligence

———

Learn from the patterns in the data coupled with an understanding of physics and chemistry

Thank You