Accelerated Materials Design and Discovery (AMDD)

An Industry-University Collaboration

Brian Storey, Toyota Research Institute

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Summary

- What is TRI?
- What materials problems are we trying to solve?
- What is TRI actually going to do?
  - Applications
  - Developing tools for AI/ML

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What is TRI?

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The New York Times

TECHNOLOGY

Toyota Invests $1 Billion in Artificial Intelligence in U.S.

By JOHN MARKOFF NOV. 6, 2015

PALO ALTO, Calif. — Silicon Valley is diving into artificial intelligence technology, with start-ups sprouting up and Google and Facebook pouring vast sums into projects that would teach machines how to learn and make decisions. Now Toyota wants a piece of the action.

Toyota, the Japanese auto giant, on Friday announced a five-year, $1 billion research and development effort headquartered here. As planned, the compound would be one of the largest research laboratories in Silicon Valley.

Conceived as a research facility bridging basic science and commercial engineering, it will be organized as a new company to be named Toyota Research Institute. Toyota will initially have a laboratory adjacent to Stanford University and another near M.I.T. in Cambridge, Mass.

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Company started in January 2016

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TRI today

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TRI mission

TRI's mission is to use artificial intelligence to improve the quality of human life.

- **Vehicle safety**
- **Mobility access**
- **Robotics**
- **Discovery in materials science**

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TRI goals

Safety

~ 1,250,000 People / Yr. Worldwide
(~ 35,000 in the US)

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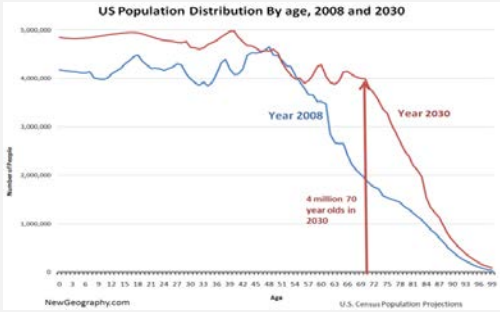
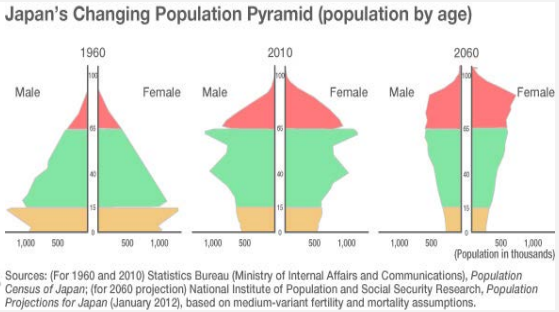
Access





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Quality of Life

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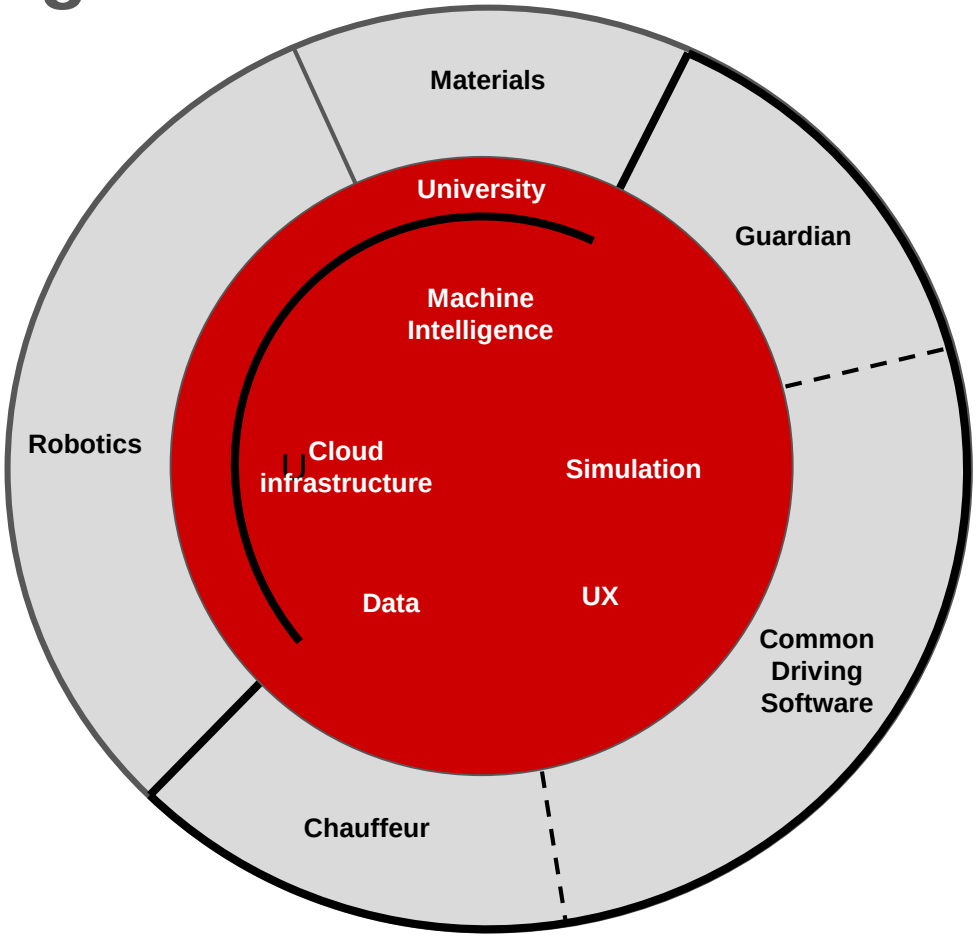
TRI R&D organization structure



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Role of simulation and data

Data gathering cars
with ordinary drivers

Millions of miles

Simulator

Billions of miles

Test cars
with professional
drivers

Millions of Miles

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What materials problems are we trying to solve?

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Materials in an AI company?

"Artificial intelligence is a vital basic technology that can… accelerate the pace of materials discovery and help lay the groundwork for the future of clean energy."

-TRI Chief Science Officer Eric Krotkov

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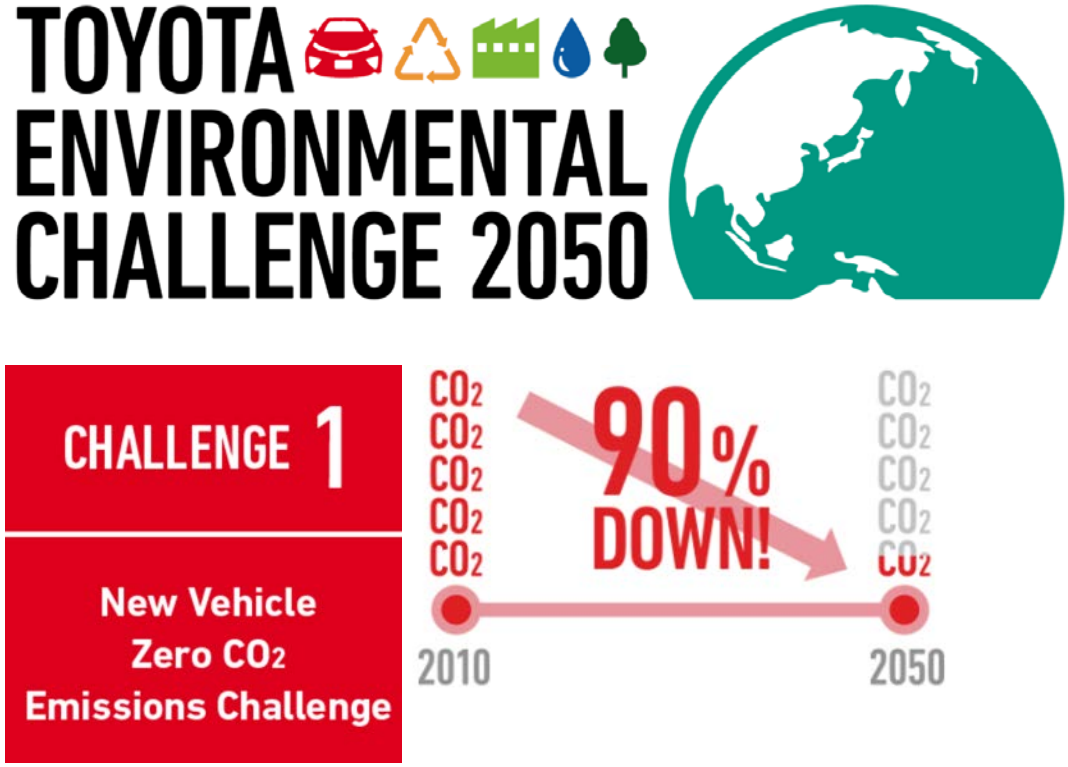
Energy storage for a new world of mobility



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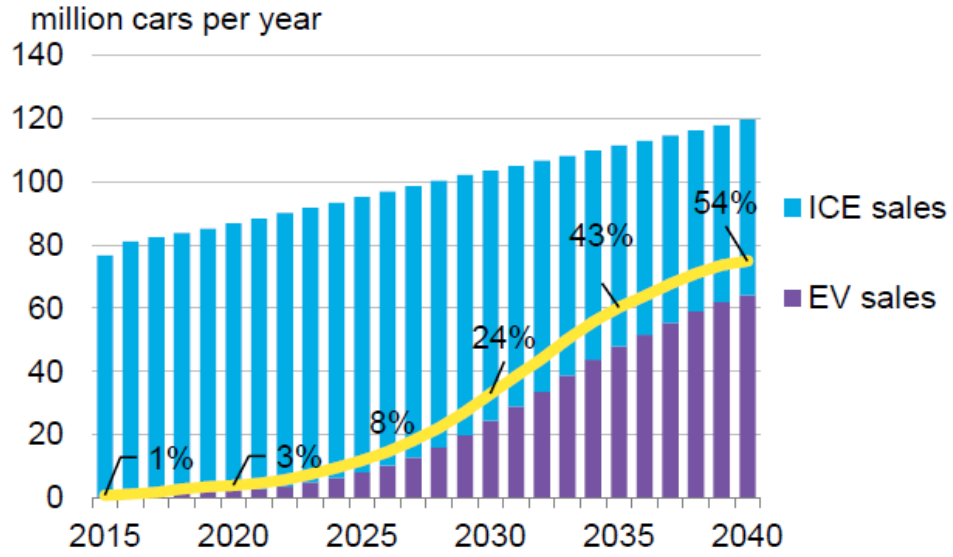
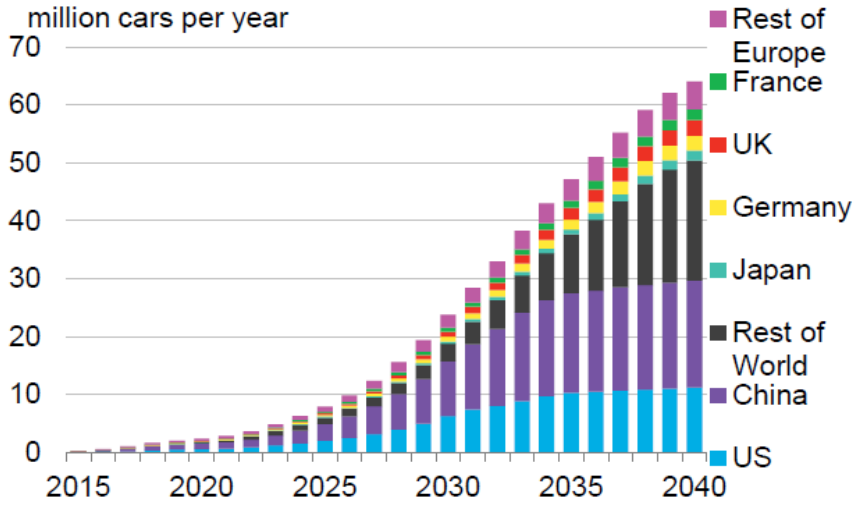
Beginning of a new era for electric cars?



Source: Bloomberg New Energy Finance



Source: Bloomberg New Energy Finance. For a detailed descriptio

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BUSINESS DAY

Germany Should Consider Electric Cars Quotas, Deputy Economy Minister Says

EUROPE

Britain to Ban New Diesel and Gas Cars by 2040

By STEPHEN CASTLE JULY 26, 2017

ENERGY & ENVIRONMENT

France Plans to End Sales of Gas and Diesel Cars by 2040

By JACK EWING JULY 6, 2017

ENERGY & ENVIRONMENT

Volvo, Betting on Electric, Moves to Phase Out Conventional Engines

By JACK EWING JULY 5, 2017

BUSINESS DAY

Tesla's First Mass-Market Car, the Model 3, Hits Production This Week

By NEAL E. BOUDETTE JULY 3, 2017

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Challenge 1: Physics and materials

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Challenge 2: Time

Materials technology	Year invented	Commercialization	Years (approximately)
Vulcanized rubber	1839	late 1850s	20
Low-cost aluminum	1886	early 1900s	15
Teflon	1938	early 1960s	25
Velcro	early 1950s	early 1970s	20
Polycarbonate	1953	about 1970	20
GaAs	mid-1960s	mid-1980s	20
GaN	1969	1993	24
NdFeB magnets	1983	late 1980s	7
Li-Ion batteries	1976	1991	15
Ferrium M54	2007	2015	8

Mulholland, Paradiso, APL Materials, 2016

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Challenge 3: Scale

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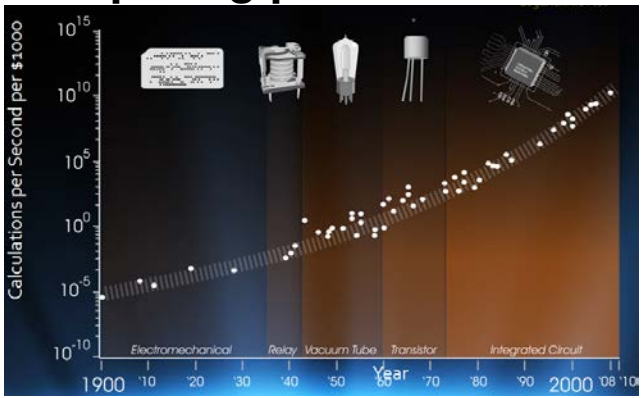
Why now?

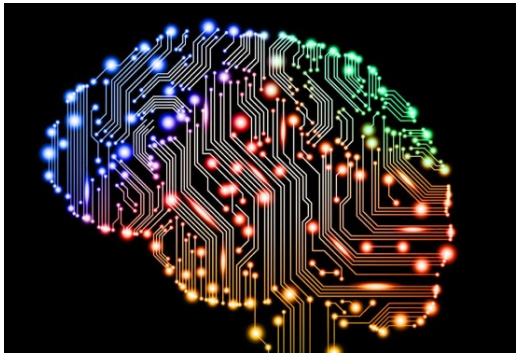
Computing power and cost



Credit: Ray Kurzweil

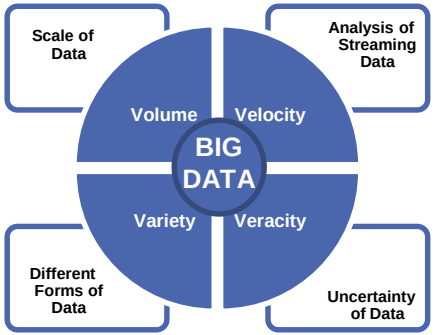
Automation

Artificial intelligence



Credit: MIT Technology Review

Big data



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Computing and simulation not enough

6 hurdles to material design (adapted from S. Shankar, Harvard)

- Characterization
- Synthesis
- Multi-scale
- Computability
- Theory
- Combinatorics

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What is TRI actually going to do?

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NEWS FROM TOYOTA

Toyota Research Institute Brings Artificial Intelligence to the Hunt for New Materials

$35 Million to Accelerate Materials Science Discovery

Projects will apply artificial intelligence and machine learning to speed development of materials for next-generation energy

March 30, 2017

Palo Alto, Calif., March 30, 2017 — The Toyota Research Institute (TRI) will collaborate with research entities, universities and companies on materials science research, investing approximately $35 million over the next four years in research that uses artificial intelligence to help accelerate the design and discovery of advanced materials. Initially, the program will aim to help revolutionize materials science and identify new advanced battery materials and fuel cell catalysts that can power future zero-emissions and carbon-neutral vehicles.

"Toyota recognizes that artificial intelligence is a vital basic technology that can be leveraged across a range of industries, and we are proud to use it to expand the boundaries of materials science," said TRI Chief Science Officer Eric Krotkov. "Accelerating the pace of materials discovery will help lay the groundwork for the future of clean energy and bring us even closer to achieving Toyota's vision of reducing global average new-vehicle CO2 emissions by 90 percent by 2050."

Initial research projects include collaborations with Stanford University, the Massachusetts Institute of Technology, the University of Michigan, the University at Buffalo, the University of Connecticut, , and the U.K.-based materials science company Ilika. TRI is also in ongoing discussions with additional research partners.

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Personnel

- 6 TRI research staff today
  - 15 is target in 1 year
- ~30 PIs
- ~80 graduate students/postdocs
  - ~ 100 by the fall

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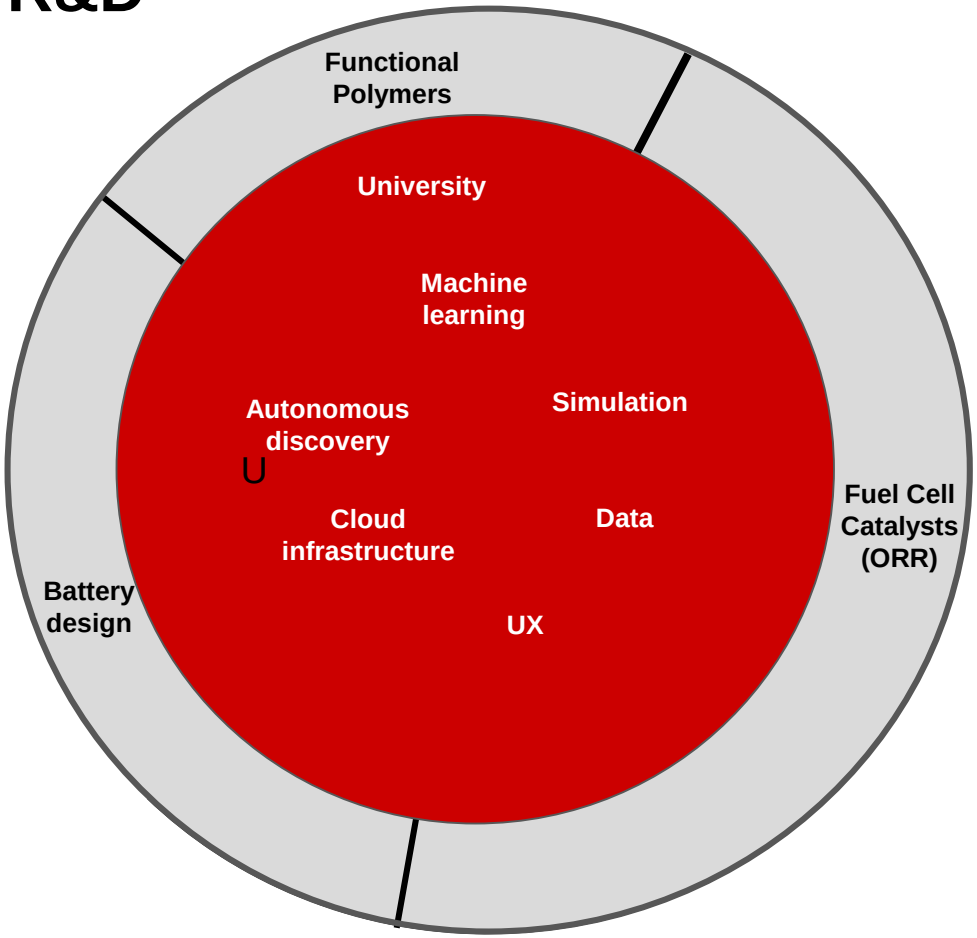
TRI materials R&D organization



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Application 1: Fuel cell catalysts

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Application 1: Fuel cell catalysts (ORR)

BUSINESS

Japan eyes 40,000 fuel-cell cars, 160 hydrogen stations by 2020

BLOOMBERG

Toyota Mirai

Amazon Finds There's Nothing Foolish in Fuel Cells

Its deal with Plug Power shows it's too early to discard hydrogen technology.

By Leonid Bershidsky

64 April 6, 2017, 12:18 PM EDT

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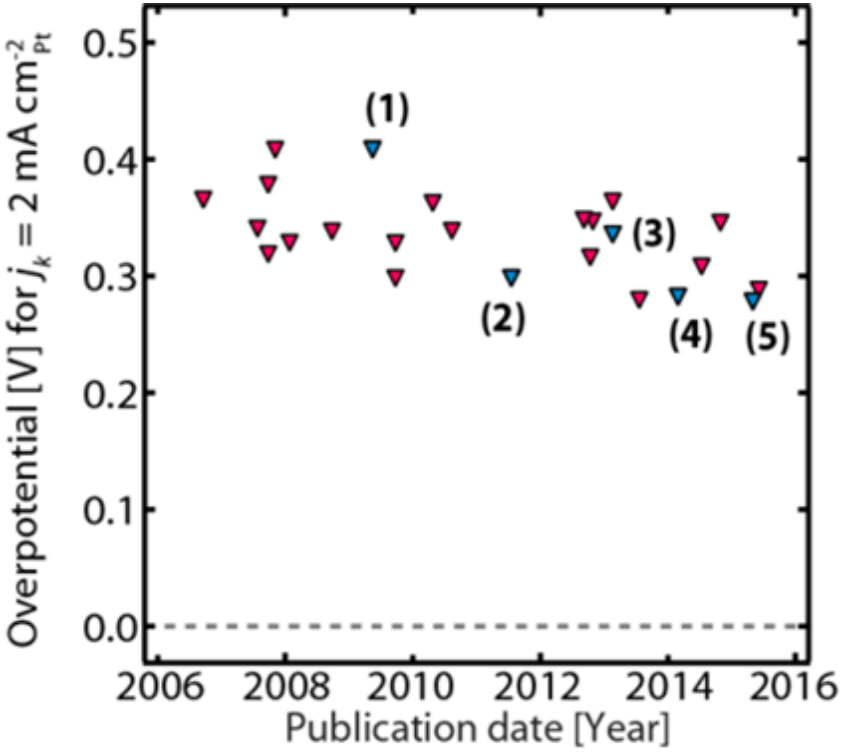
ORR: Need for a new approach



Vojvodic, Nørskov, Natl. Science Review (2015)
Montoya, Vojvodic, Nørskov (2015)

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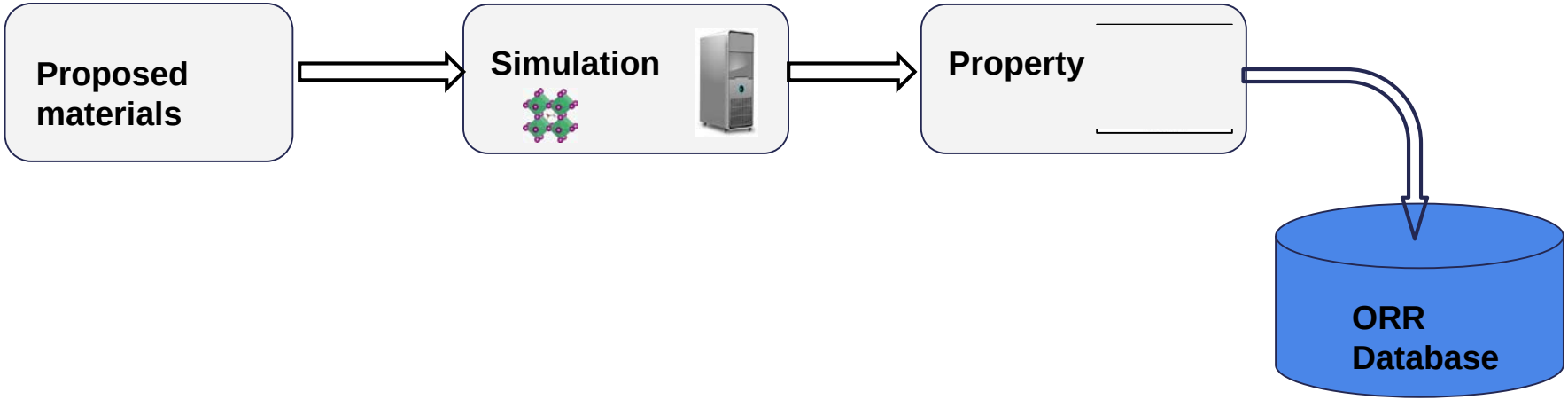
Catalysis simulation database



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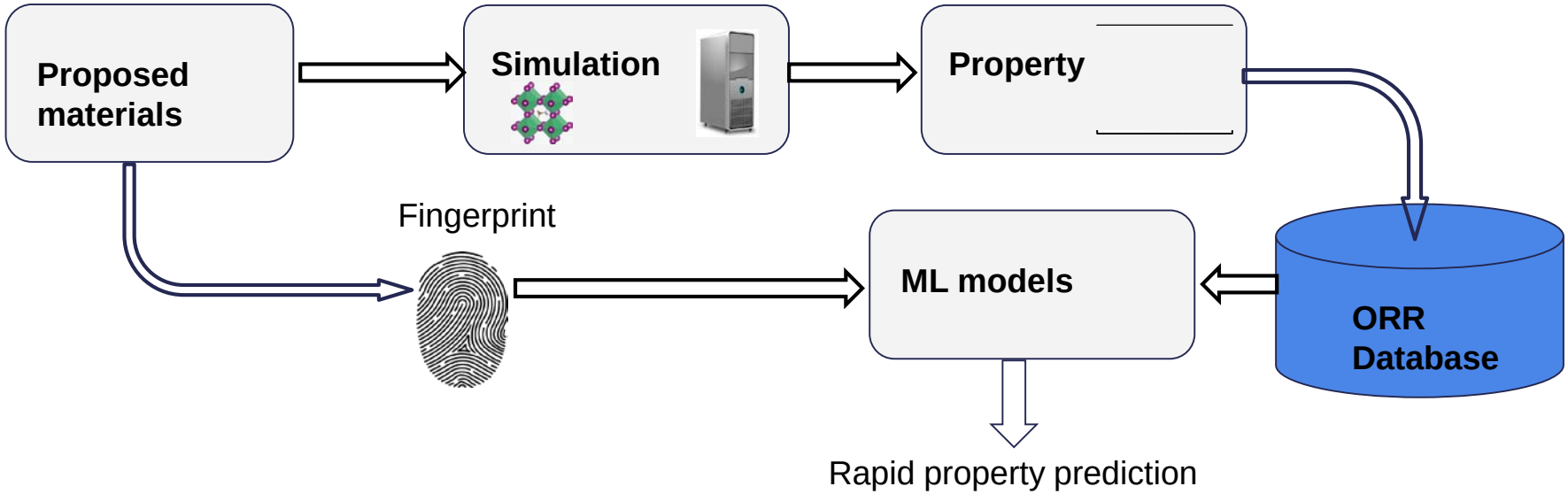
ML short cut



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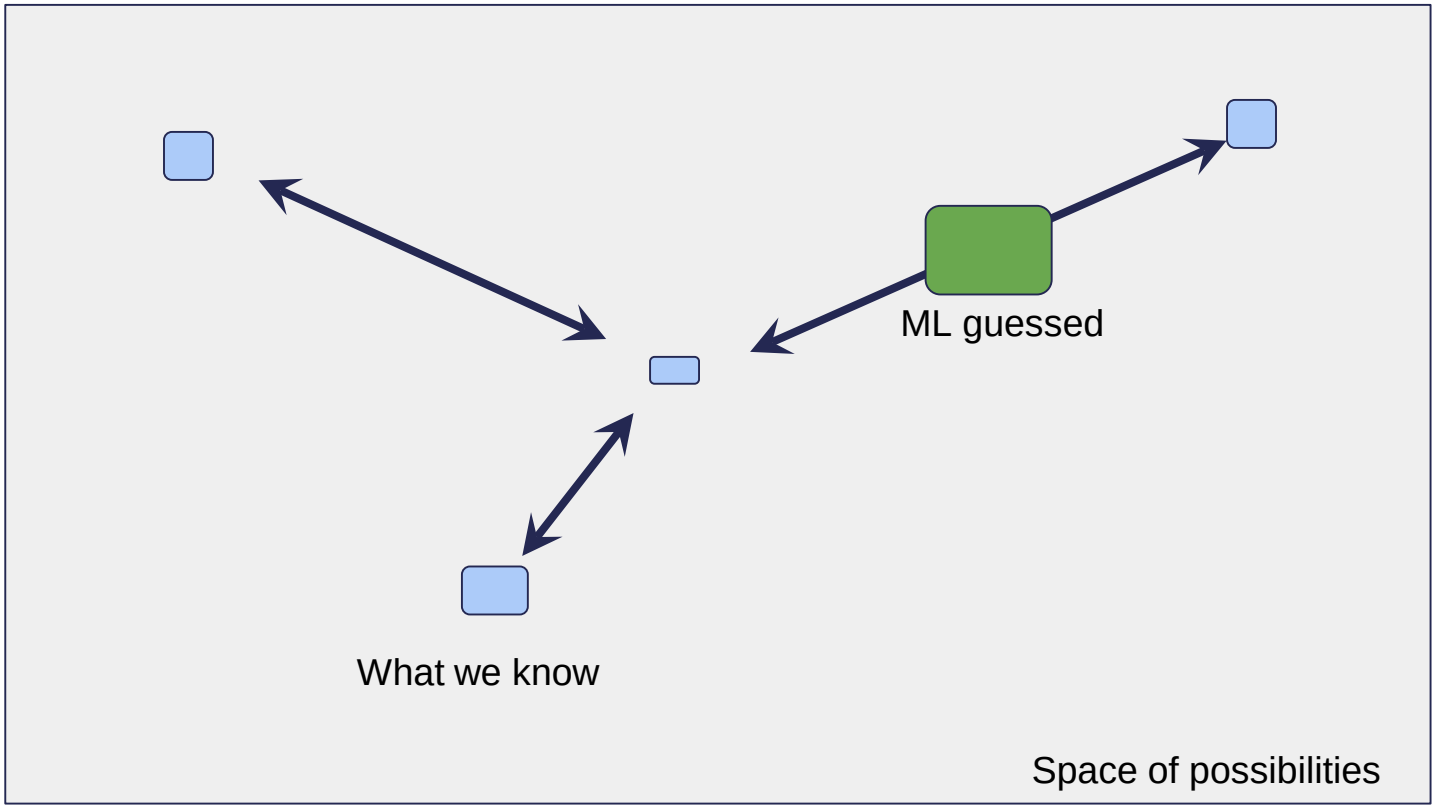
Interpolating materials space



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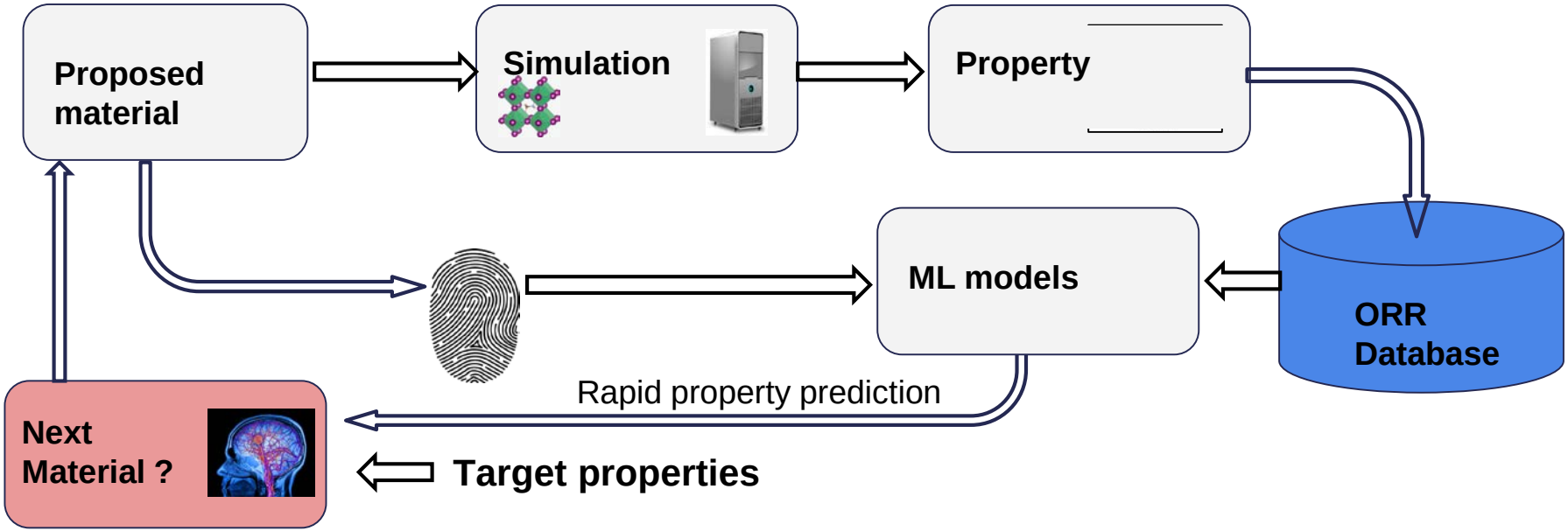
Automated feedback



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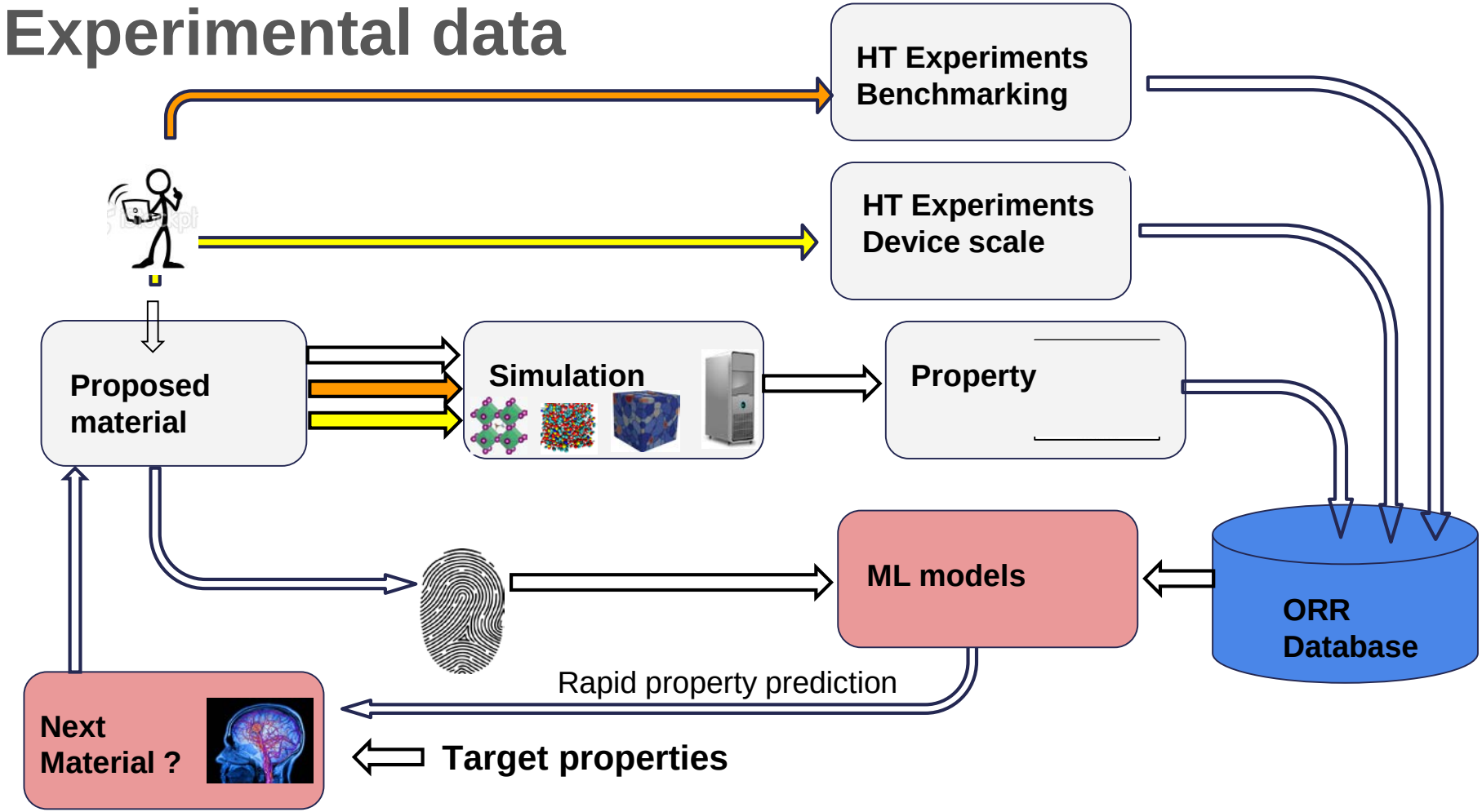
Experimental data



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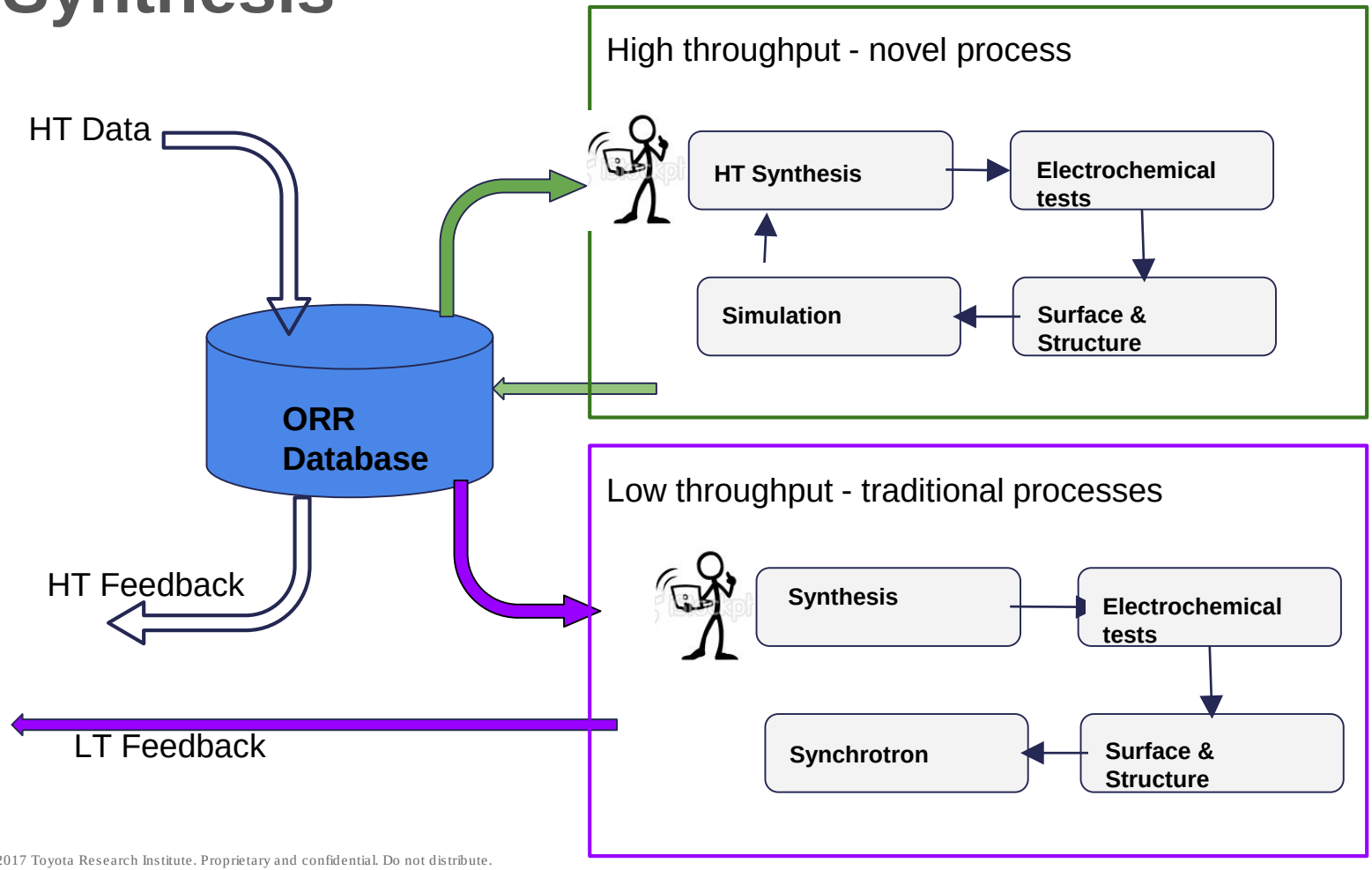
Synthesis



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AI for materials discovery

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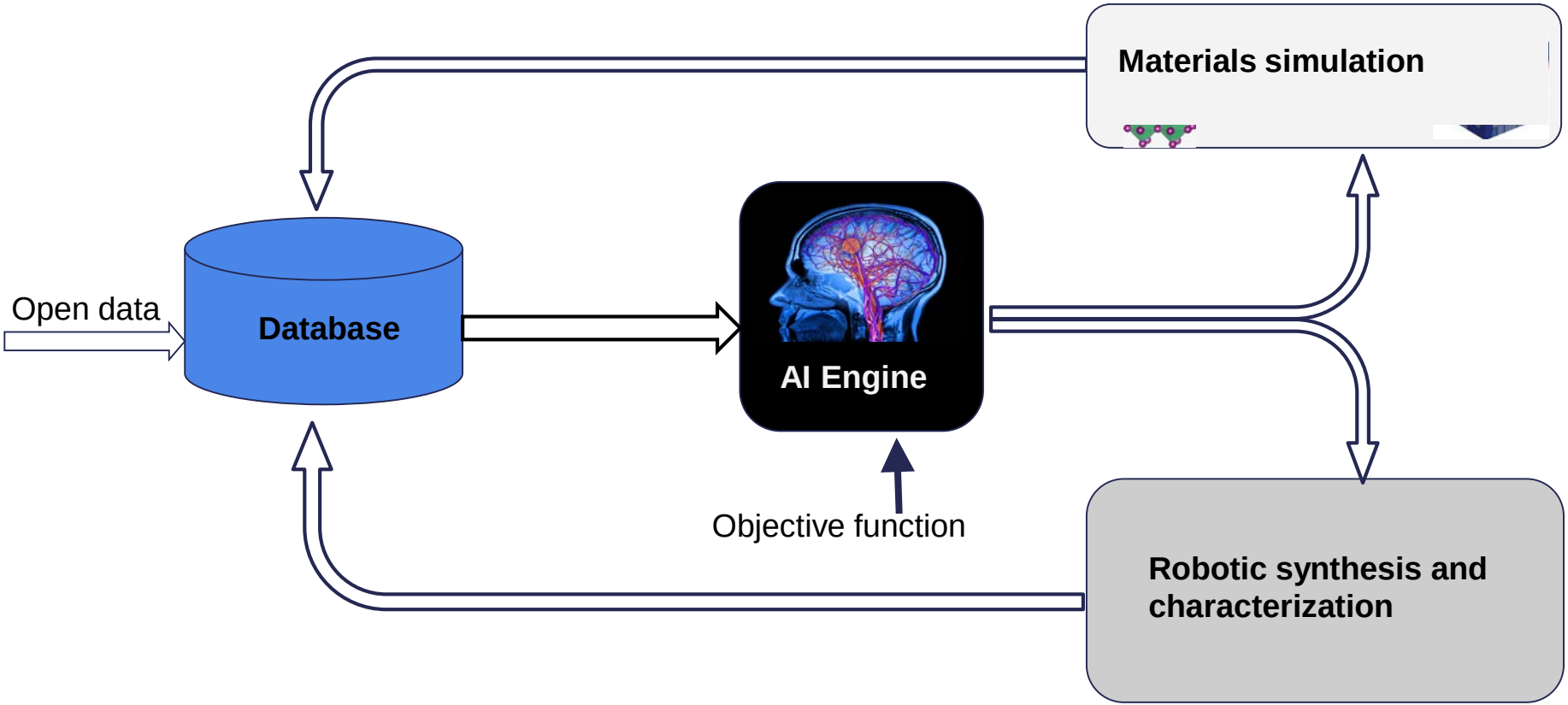
AI optimization dream



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Reasons to remain skeptical

”... the possibility of machine aided scientific discovery. We believe the techniques underpinning AlphaGo are general purpose and could be applied to a wide range of other domains, especially those with clear objective functions that can be optimized and environments that can be accurately simulated, allowing for efficient high-speed experimentation. “ Demis Hassabis, CEO Deep Mind.

Most materials problems

- Don’t have clear objective functions
- Can’t be accurately simulated
- Don’t have rules that are easily encoded

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Final thoughts

- An exciting time for the field.
- Pharmaceutical industry offers both inspirational & cautionary tales.
- A compound is not a material. A material is not a system.
- AI is getting good at doing things people do readily (recognize images, language processing, driving a car)… but can it solve problems people can’t?

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