Beating Edison with AI, Quantum and Robots

Accelerating Discovery

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Mikael Haglund
IBM

‘Results! Why, man, I have gotten a lot of results! I know several thousand things that won’t work.’

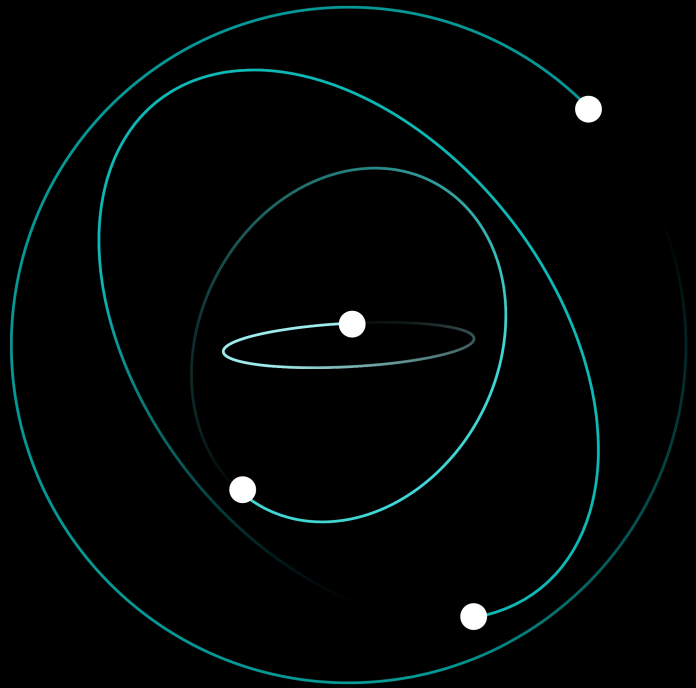
/Thomas Edison

The urgency of science has never been stronger than it is now.

We must accelerate the process of discovery to address systemic challenges.

New discoveries nearly all rely on some version of the scientific method

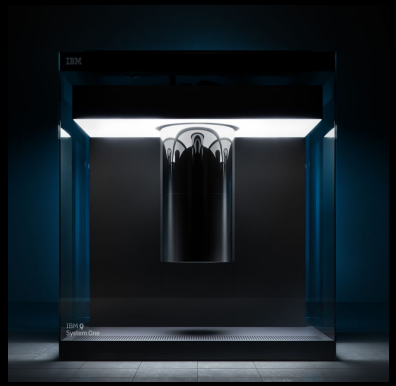
1. Study
2. Hypothesize
3. Test
4. Iterate



The accelerated discovery cycle

The use of AI will consolidate all of humanity's knowledge on a specific topic.

Traditional and quantum simulations will cover the knowledge gaps.



The corresponding data can be used to create inference models to generate hypotheses and automate their testing.

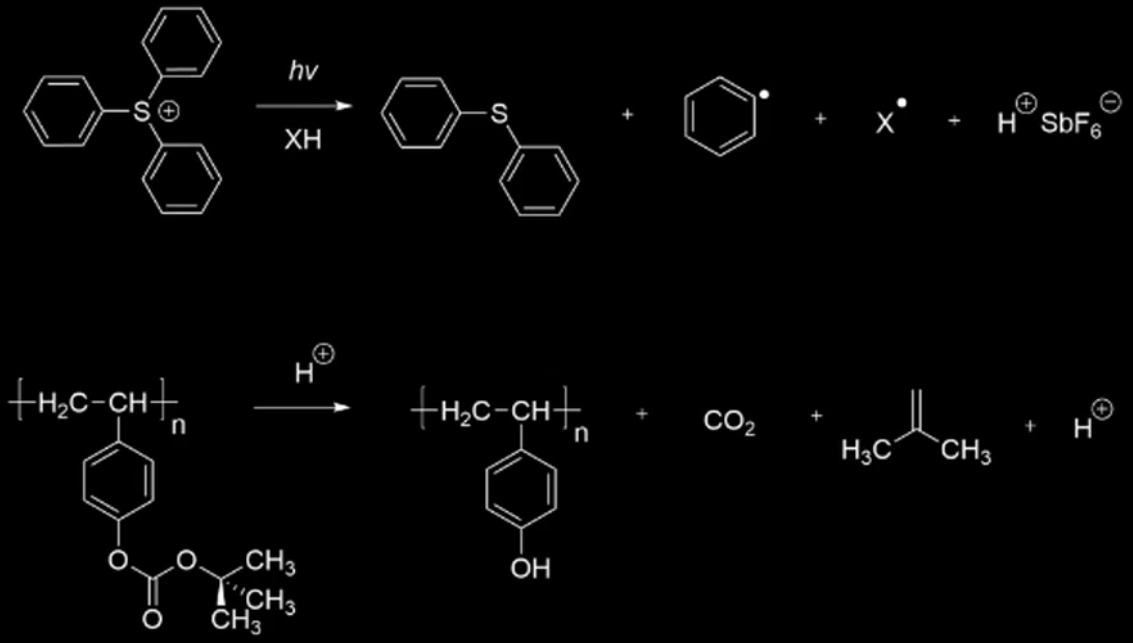
This composable infrastructure of emerging technologies will be enabled and managed by the hybrid cloud.

The process of material design and discovery

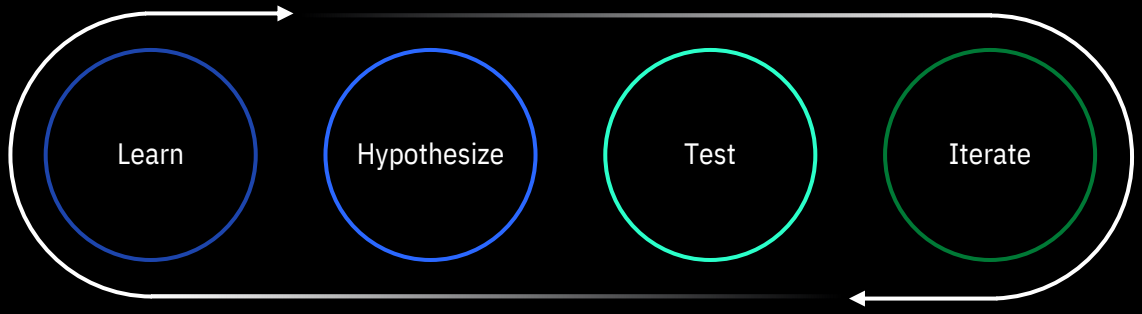
It typically takes roughly 10 years and upwards of $10 - $100 million to discover one new material.

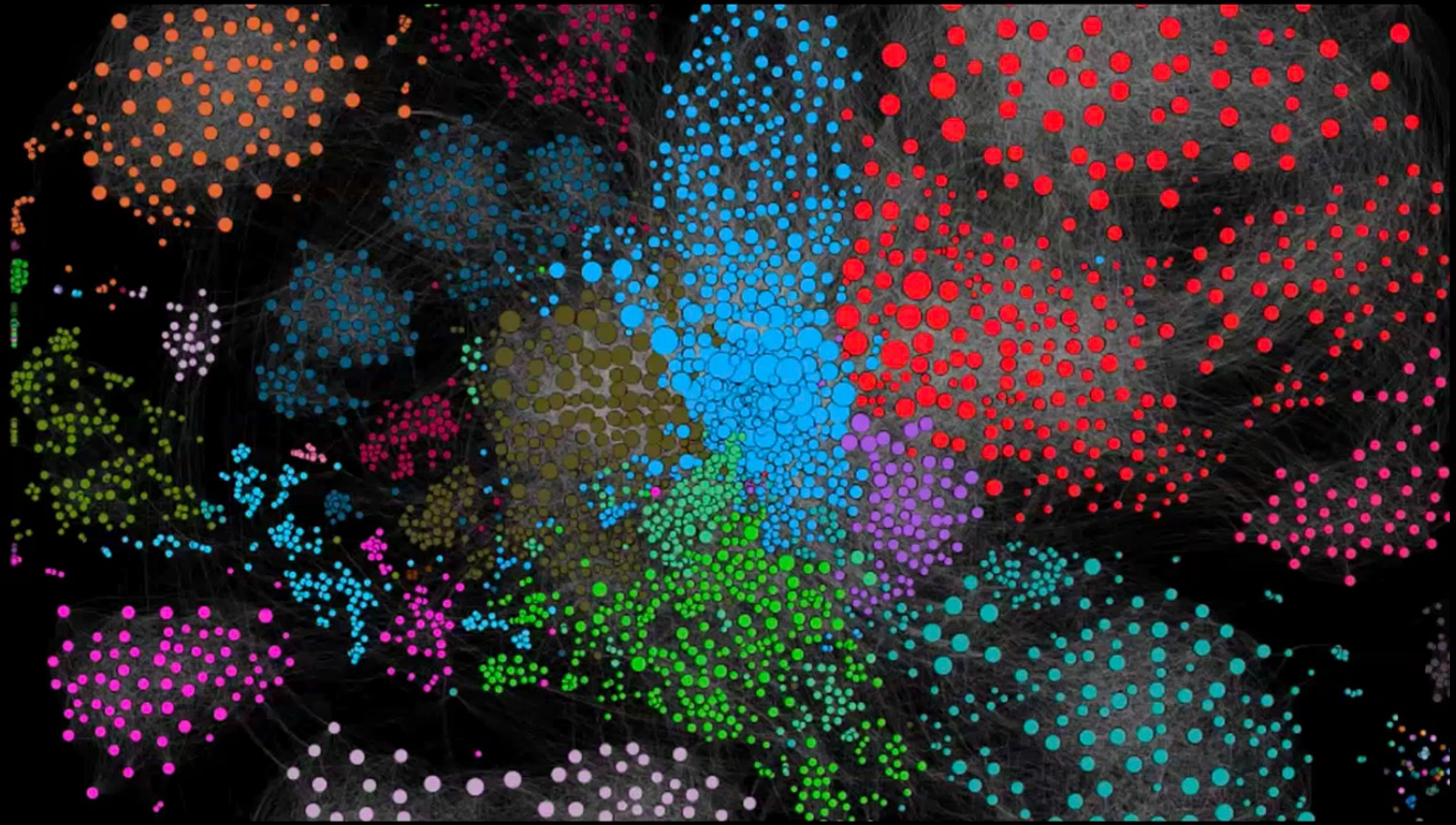
We aim to cut down both years and cost by 90%

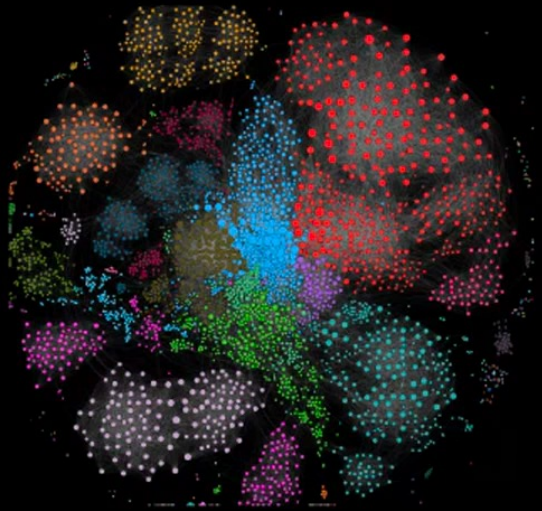
A chemically amplified photoresist example, developed at IBM in 1983



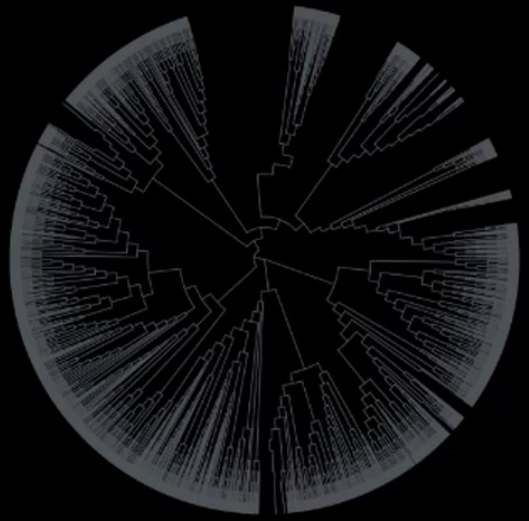
We apply the supercharged scientific method







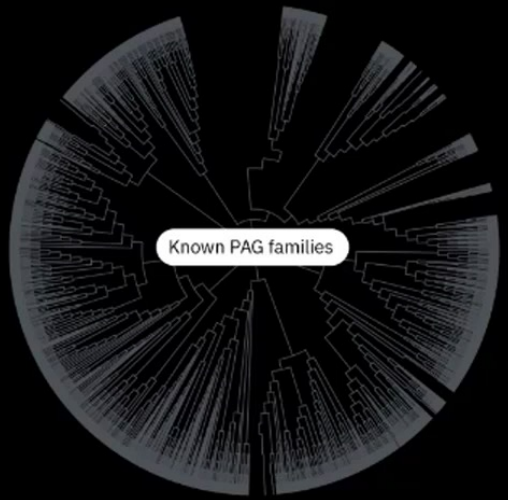
Known PAG chemistry space



PAG Family Graph

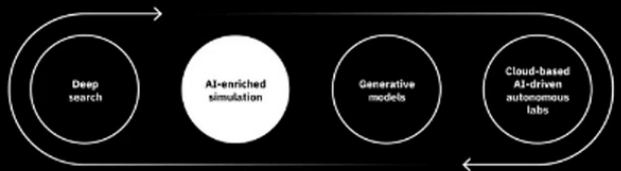
We start by discovering what is known about PAGs using deep search.

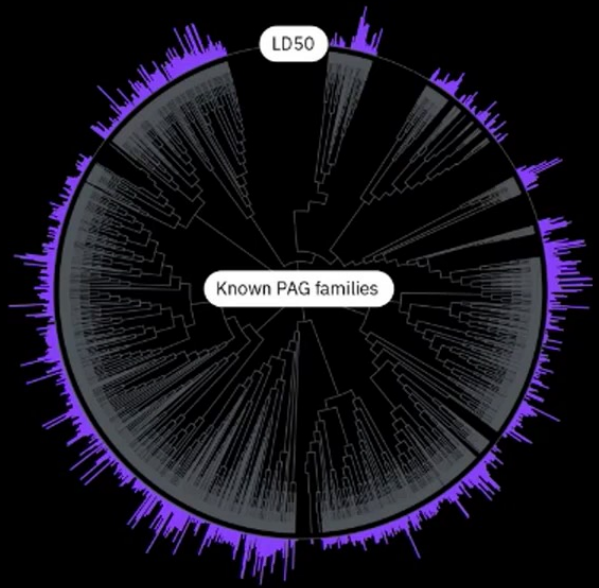
→ 6,000 patents/papers consisting of about 60,000 pages is ingested in about 1 hour .



We then augment with simulation.

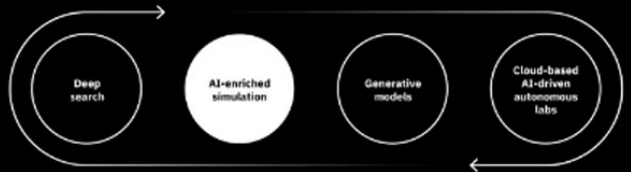
→ Computed property values associated with toxicity.

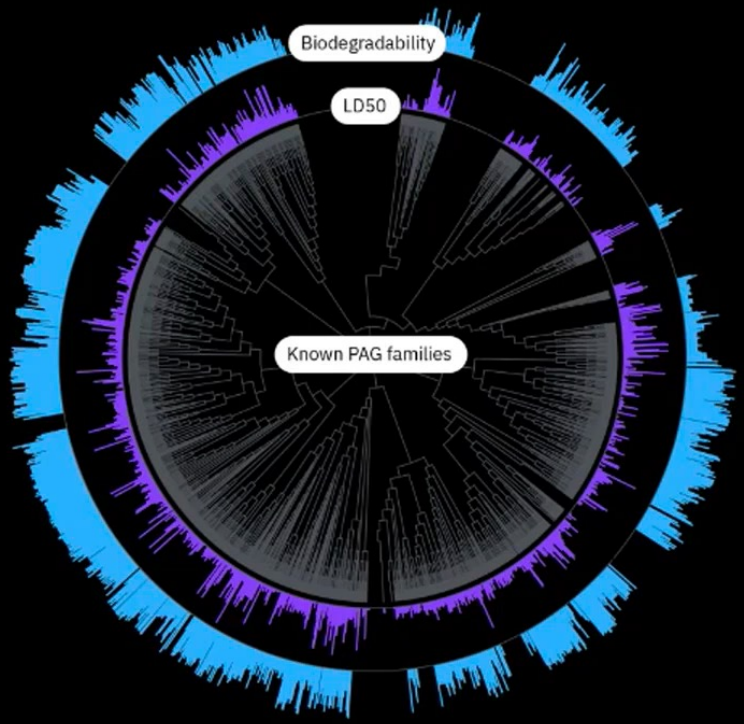




We then augment with simulation.

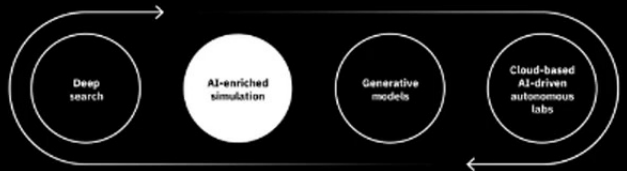
→ Computed property values associated with Persistence.

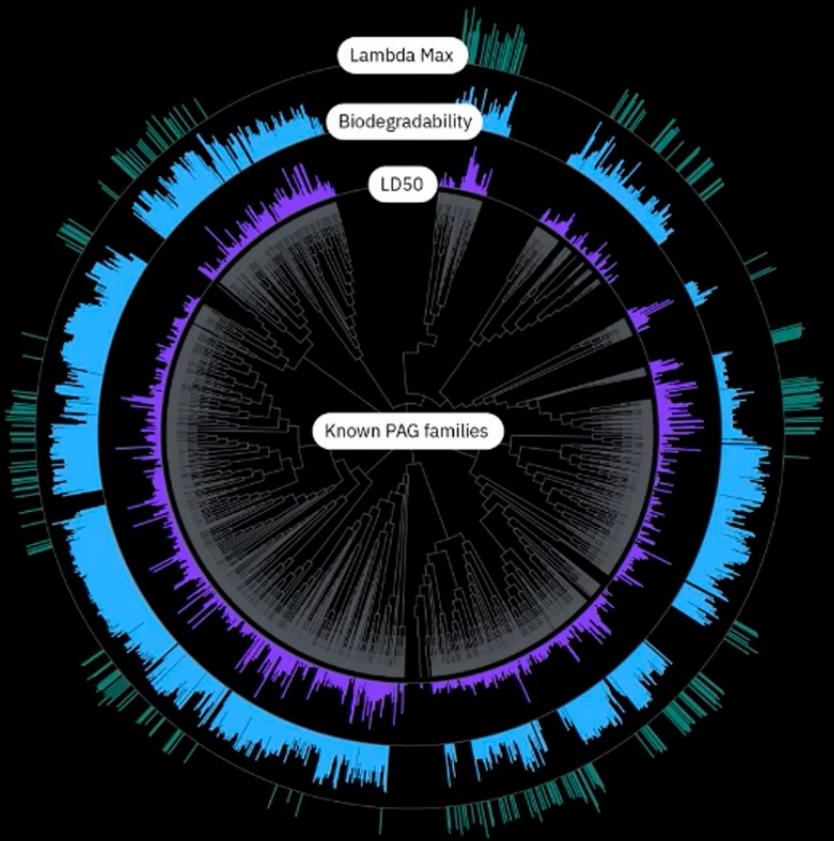




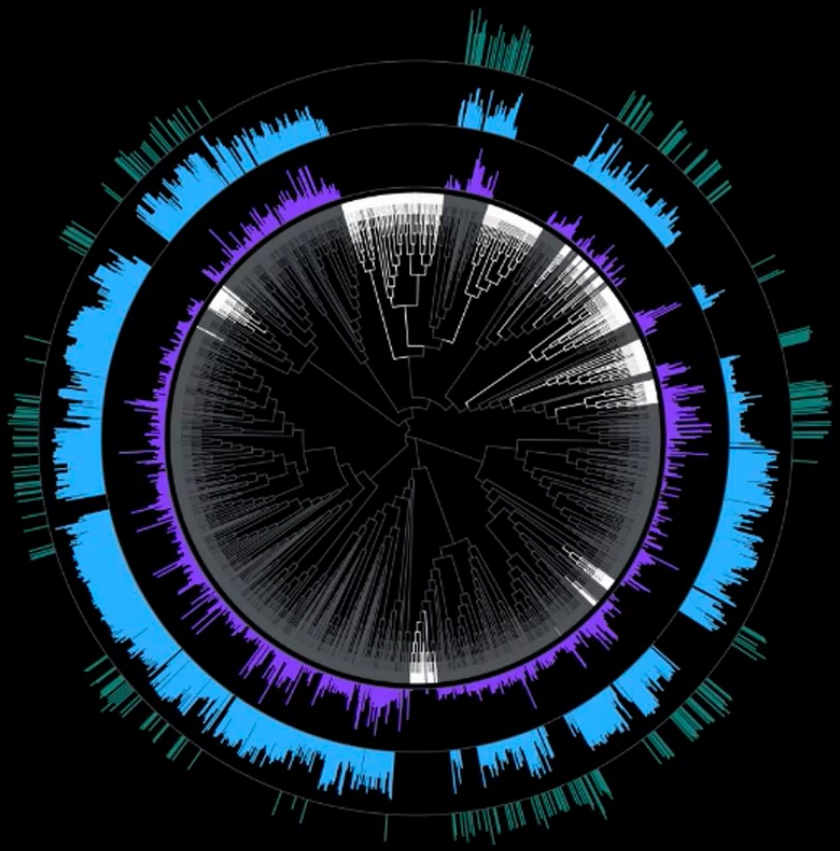
We then augment with simulation.

→ Computed property values associated with photochemistry.



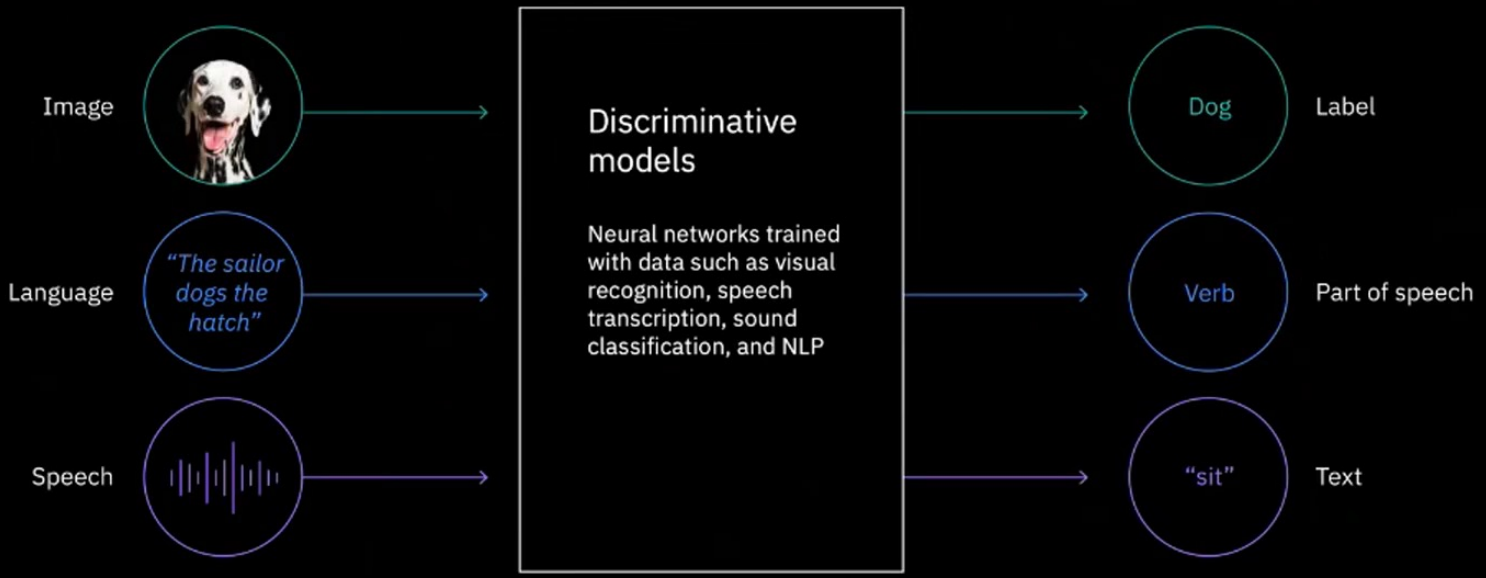


We then expand with generative models.

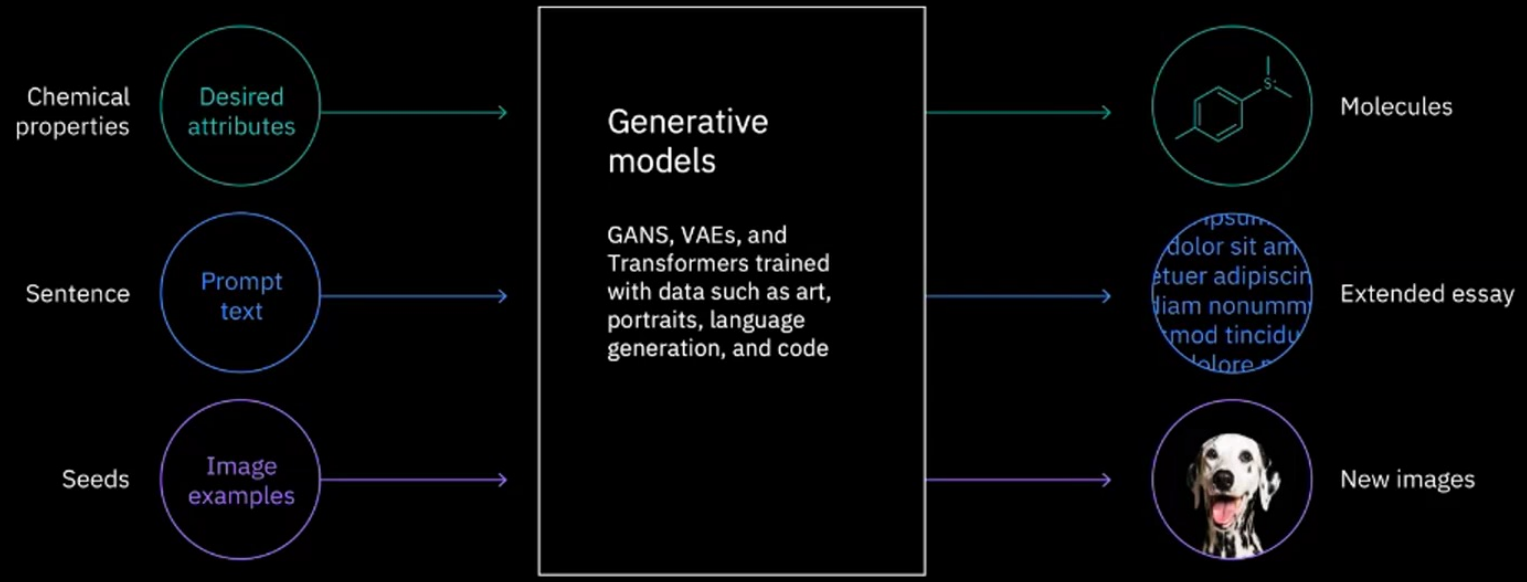


The power of generative models move AI from discriminator to generator

Discriminative models



Generative models



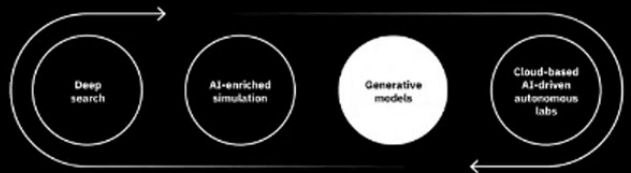
The awesome team!

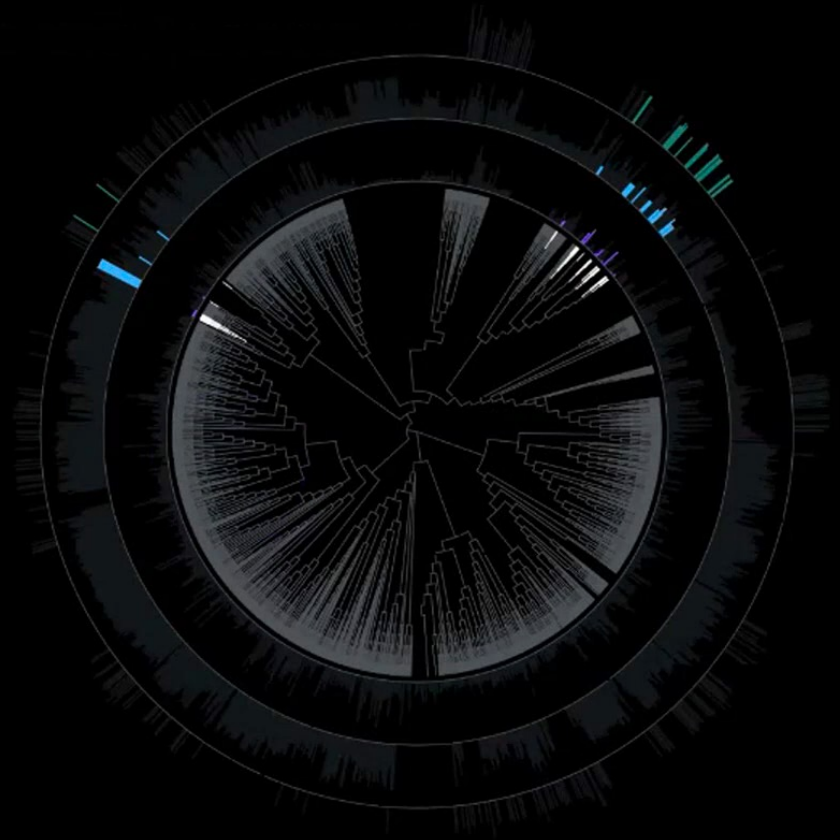
https://thispersondoesnotexist.com/image

Filter with human expertise + AI.

→ Result

Newly discovered materials predicted to have increased sustainable qualities for PAGs.





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