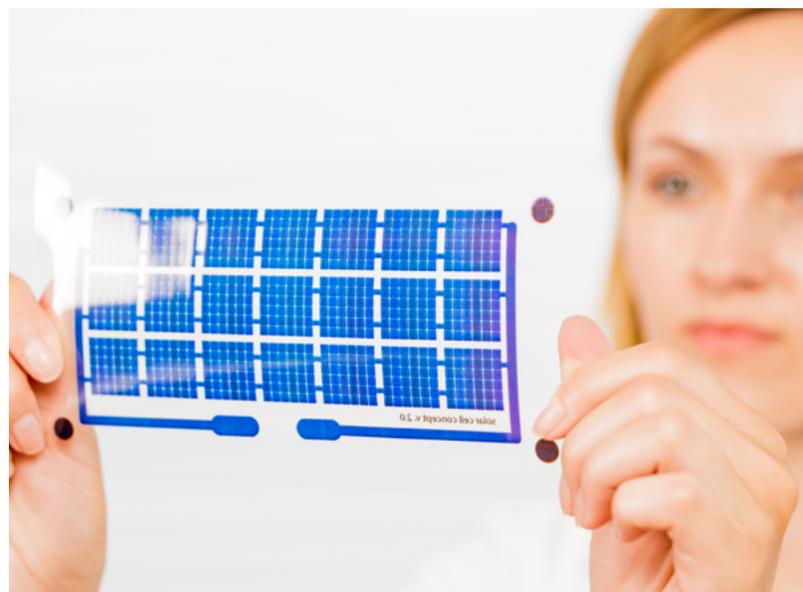CITRINE
INFORMATICS

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MACHINE LEARNING ACCELERATES MATERIALS DISCOVERY

PANASONIC DEVELOPS NEW, PATENT PENDING ORGANIC SEMICONDUCTOR MOLECULES WITH CITRINE'S AI PLATFORM

CITRINE
INFORMATICS

Panasonic

EXECUTIVE SUMMARY

IP GROWN
PATENTS PENDING ON HIGH MOBILITY THIEONOACENES

PERFORMANCE IMPROVED
25% INCREASE IN HOLE MOBILITY CALCULATED

TIME SAVED
ONLY 196 DFT CALCULATIONS PERFORMED ON > 1 MILLION CANDIDATES

NEW INSIGHTS
INTO HOW MOLECULAR TOPOLOGY AFFECTS HOLE MOBILITY

"This work demonstrates the utility of using the sequential learning methodology to design experiments for the discovery of novel materials."

Nobuyuki Matsuzawa,
Panasonic

THE CHALLENGE

The internet of things requires flexible, lightweight and inexpensive semiconductors. Panasonic is already using organic semiconductors for IOT applications, but they needed a way to reduce processing costs while also increasing performance. Heteroacenes are a molecular class of organic semiconductor that are soluble in organic solvents, enabling cheap spin-coating techniques. But there are millions of them, far too many to exhaustively survey experimentally or computationally. Panasonic and Citrine combined their expertise to meet this challenge.
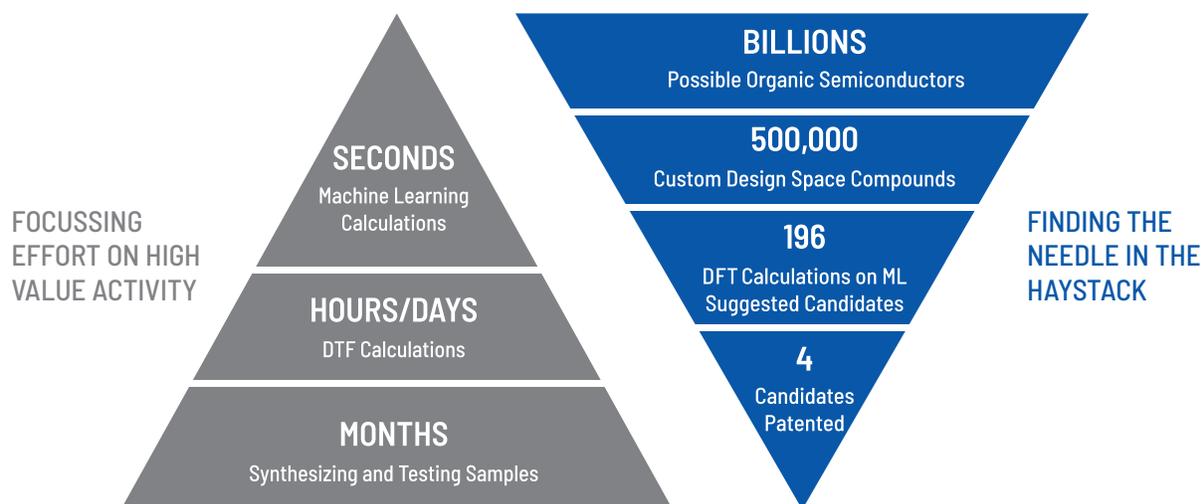
THE APPROACH

Citrine created a list of feasible molecular candidates (design space) based on the Panasonic scientists' intuition and knowledge of molecular design principles. In particular, the Citrine Platform's ability to interpret and analyze chemical formulas – especially the representation of fused rings – was essential for this step.

Next, Panasonic's molecular simulation team combined their expertise in physics-based Density Functional Theory (DFT) and Molecular Dynamics (MD) simulations with the AI capabilities of the Citrine Platform. MD and DFT are less time-consuming than synthesizing and testing physical samples, but they still take days. Citrine's AI was able to focus the Panasonic team's efforts on simulations with the highest likelihood of success.

THE RESULTS

With the help of Citrine, Panasonic designed a molecule with 25% higher hole mobility than they had previously seen, in record time. This compound and 3 others discovered via this AI-driven workflow are now patent pending, and Panasonic plans to synthesize them in the near future.

In addition to reduced R&D time and cost, the Panasonic team gained insight into the effects of molecular structure and fused thiophene rings on hole mobility. This scientific knowledge is now captured in the machine learning models and can be reused on future projects.

FOCUSSING EFFORT ON HIGH VALUE ACTIVITY

SECONDS
Machine Learning Calculations

HOURS/DAYS
DTF Calculations

MONTHS
Synthesizing and Testing Samples

BILLIONS
Possible Organic Semiconductors

500,000
Custom Design Space Compounds

196
DFT Calculations on ML Suggested Candidates

4
Candidates Patented

FINDING THE NEEDLE IN THE HAYSTACK

FIND OUT MORE

ABOUT CITRINE INFORMATICS

Citrine Informatics is the award-winning materials informatics platform for data-driven materials and chemicals development. It won the 2017 World Materials Forum Start-up Challenge, the 2018 AI Breakthrough award as the "Best AI-based Solution for Manufacturing", and 2020 Cleantech 100 honors. The Citrine Platform combines smart materials data infrastructure and Artificial Intelligence, which accelerates development of cutting-edge materials, facilitates product portfolio optimization, and codifies research IP; enabling its reuse and preventing its loss. Citrine's customers include Panasonic, BASF, LANXESS, and some of the biggest and most respected names in the materials and chemicals industry in Asia, North America, and Europe. For more information visit our website at Citrine.io, or contact us at +1 650-276-7318.