CASE STUDY

MATERIALSIN

Data-Driven Discovery

PRECURSOR DISCOVERY FOR NEXT-GENERTATION LOW-K DIELECTRICS

Customer:

Global Semiconductor Manufacturing Equipment Company

Outcome:

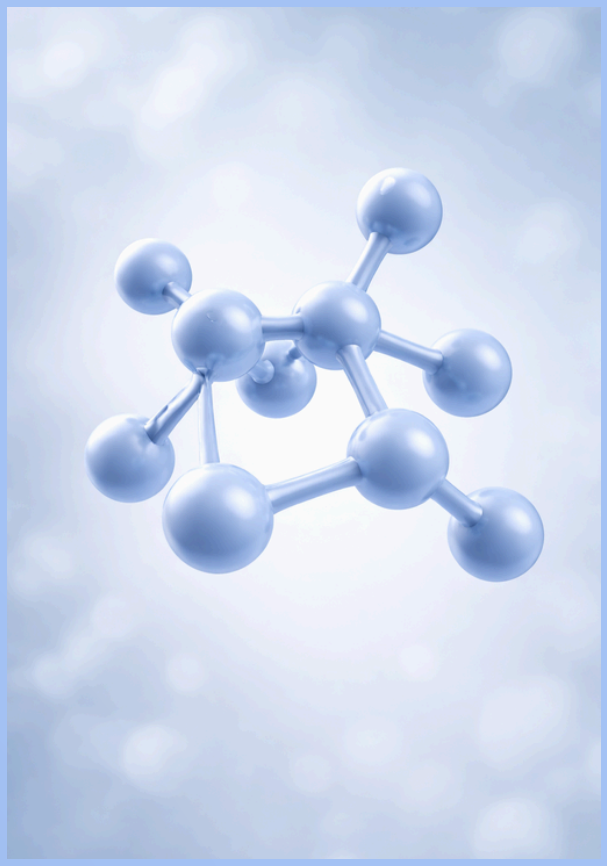
materialsIN rapidly generates scientifically-grounded recommendations and shortlists of precursor candidates for experimental evaluation in advanced process development

Executive Summary

Data-Driven Precursor Discovery Strategy

materialsIN's innovative approach leverages data-driven insights to transform precursor discovery for advanced low-k dielectrics, enhancing efficiency in semiconductor manufacturing processes and paving the way for next-generation materials.

By utilizing machine learning and materials informatics, this method supports rapid identification of viable vapor-phase precursor candidates, addressing the challenges of traditional experimentation and ultimately accelerating the commercialization of advanced microelectronic devices.



The Challenge

Identifying Vapor-Phase Precuror Candidates for Experimental Synthesis Evaluation

Advanced low-k dielectric materials are crucial for enhancing microelectronic device performance, yet the synthesis pathways for suitable vapor-phase precursors remain underexplored and complex. Effective identification is essential for innovation.

A fundamental barrier to experimental progress was the identification of suitable vapor-phase precursor molecules that satisfy stringent, often competing, constraints: sufficient volatility, thermal stability, controlled surface reactivity, and compatibility with self-limiting ALD/MLD reaction cycles. Traditional trial-and-error precursor discovery is slow, expensive, and high-risk, particularly when exploring unfamiliar multi-metal or ligand-mediated reaction spaces.

materialsIN addresses these challenges by employing data-driven methods to streamline the precursor discovery process, enabling semiconductor manufacturers to efficiently navigate the intricate requirements of modern material synthesis.

The Approach

materialsIN applied its proprietary materials informatics and machine-learning methodology to develop a systematic precursor screening and ranking framework grounded in the foundational principles of organic chemistry.

Key Points

SCREENING

Systematic selection of potential chemical precursors from millions of compounds, enhancing discovery efficiency.

PATHWAYS

Identification of successful processing and synthesis pathways through a data-fusion system, linking relevant databases.

UNCERTAINTY

Uncertainty-informed decision-making tools that harness large models to explore alternative reasoning paths for materials synthesis.

AI PLATFORM

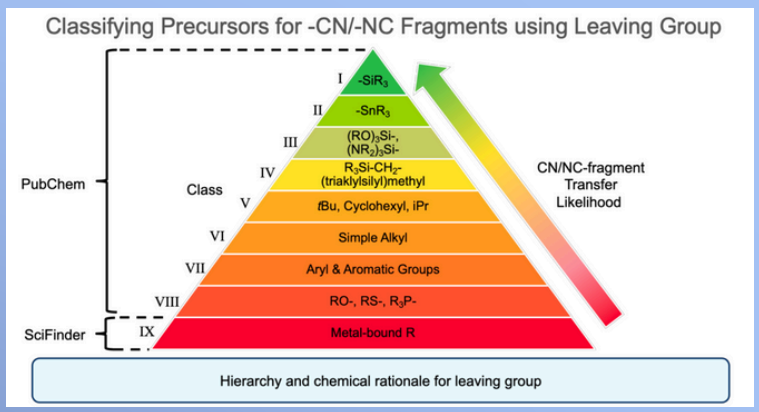
Development of a science-informed AI platform that refines results interpretation, balancing speed with decision-making.

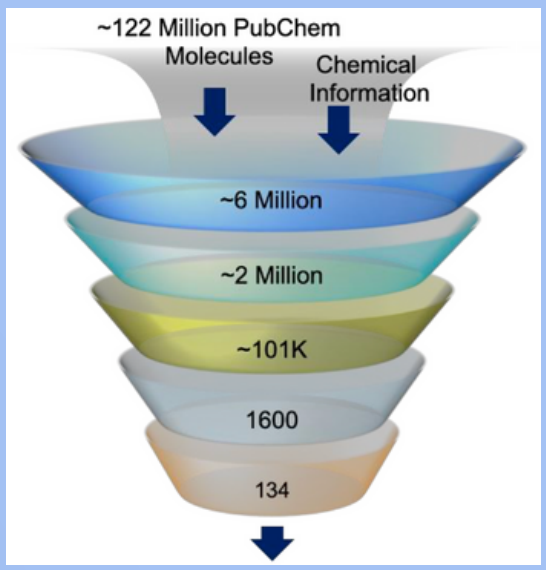
The Results

materialsIN delivered a scientifically defensible, vendor-accessible precursor shortlist, along with a transparent selection logic linking molecular features to process feasibility.

Highlights:

- Ranked library of candidate vapor-phase precursor molecules
- Chemically diverse screening subset suitable for immediate experimental testing
- Mechanistic reaction-pathway map guiding experimental sequence design
- Closed-loop informatics framework enabling continuous refinement





The Impact

The engagement demonstrates how materialsIN's materials-informatics platform accelerates precursor discovery for advanced semiconductor process development

COMPRESS TIMELINES

Acceleartes precursor identification by 50%

COST CUTS

Mnimize trail-and-error experimentation leading to substantial cost saving by 50%

DATA DRIVEN LOGIC

Interpretable selection logic, empowering teams to make informed decisions

LINKS MODELING

integrates modeling and experimentation, offering data-guided insights that streamline the validation process

materialsIN Inc.

Contact Information:
Frits Abell, CEO
Frits@materialsin.com / 646.228.1673

materialsIN.com