# Accelerating Materials Discovery

**Through Advanced Metrology and Machine Learning** 

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- 1. Introduction: Accelerating Materials Innovation
- 2. Multi-Technique Metrology Approach
- 3. Automatic Data Analysis and Database Creation
- 4. Modeling and Machine Learning

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## **Introduction: Accelerating Materials Discovery**

How long does it take to develop materials from discovery to production?



J.P Correa-Baena, Joule 2, 1410 (2018)

How can we accelerate materials discovery?

- Advanced Metrology: Increased Resolution and Automation
- Automated Data Analysis: Database Creation
- Machine Learning: Separate Trends, Find New Compositional Spaces

# **Accelerating Materials Innovation: High Throughput Experimentation**

High Throughput Process



Advanced Characterization



#### **Processing Systems**

- Dry: ALD, CVD, PVD, etch
- Wet: Clean, Etch, Deposition

#### Lithography & Etch

- Contact lithography, coat, exposure, develop & etch
- Oxide and metal etch



Physical & Optical Characterization

- XRF, XRR, XRD, XPS
- Ellipsometry, UV-VIS-NIR, FTIR, Raman
- Optical microscopy, SEM, AFM, profilers, contact angle



#### **Electrical Characterization & E-test**

- C-V, I-V P-V & parameter extraction
- Leakage, line resistance, contact resistance, capacitance
- V<sub>bd</sub>, TDDB
- Pulsed switching: I<sub>on</sub>, I<sub>off</sub>, data retention (eg. NVM)
- Variable temperature

Data Analysis & Mechanism Understanding

#### **IMI Informatics SW**

- Substrate management (R&D MES)
- Automated data collection & analysis
- Database creation consolidating Process and Metrology Data



#### **Machine Learning**

- Separate Trends
- Create Predictive Model



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## **Challenging Materials Development Requires A Wide Multi-Technique Metrology Approach**



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# **Highly Automated Electrical Test and Data Analysis**

#### Semi-Automatic Prober



- 200mm, 300mm
- Thermal (-50 to 300C)
- GPIB Automation

#### Advanced Characterization Instruments





- State-of-the-Art Instruments Fully Automated (GPIB, Serial)
- In-house Driver Software

### **Etest Automation**



 Framework automates communicates with tools and automates e-test.

#### Informatics



- Product/Substrate Definition
- Operations/Workflow Management
- DOE, Data Presentation/Export

### Data Analysis



- Device Level Analysis Tables
- Automated
  Reports/Summaries
- Device Performance, Correlation with Process Parameters, etc...



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# **Automated Data Analysis and Database Creation**



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# **Modeling of Properties Allows Understanding Compositional Trends**



Phenomenological Models Allow Compositional Targeting



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# **Machine Learning To Reveal Trends and Understand Tradeoffs**



### Conclusions

### **Accelerating Materials Discovery Requires:**

- High Throughput Fabrication and Metrology
- Automated Data Collection, Analysis and Database Creation
- Mechanism Understating using Modeling and Machine Learning