Enthought

What Materials Informatics Looks Like in the Modern R&D Lab

Industry success now more than ever is being dictated by the ability to continuously develop innovative new materials and chemicals. **Materials Informatics** (MI) is the modern approach to materials discovery and product development that is grounded in data-driven strategies and advanced computational techniques. MI combines elements of materials science, data science, and scientific computing to develop new materials faster, cheaper, and more efficiently.

Integration of AI and ML into workflows to increase efficiency and speed.

Traditional R&D processes involve time-consuming and resource intensive trial-and-error approaches. MI techniques can significantly streamline research processes through optimized workflows for greater efficiency and speed. With AI and machine learning (ML)-driven modeling, researchers can predict material properties and behaviors, taking a more efficient path in research and product development. This leads to a reduction in costly and lengthy trial iterations, expediting the overall research timeline and time to market.

R&D scientists with strong digital skills in addition to domain expertise.

The modern lab is data-driven and scientists must have strong digital skills to turn data into a competitive advantage. Scientists trained in AI/ML and data analytics can transform product development workflows to make them far more productive. With digital proficiency, they can create data-driven research methodologies, optimize experimental design, and innovate faster than otherwise possible. R&D leadership should invest in cultivating digital leaders in their labs to drive innovation and increase productivity.

Flexible and scalable digital tools that enable scientific innovation.

The complexities of scientific data and processes require digital tools that are flexible and adaptable. MI tools should not only be purpose-built to understand how researchers use scientific data, they should be flexible to adapt to the iterative nature of experimentation itself. Whether dealing with complex materials characterization data or exploring novel materials systems, the solution must adapt to the scientific discovery process as well as seamlessly scale with constant new and unique challenges. Labs need a secure yet flexible R&D platform with a clean, unified interface to access all their data, no matter where it's stored, analyze data using familiar tools, seamlessly share assets with colleagues, and build and deploy custom MI applications with minimal IT overhead.

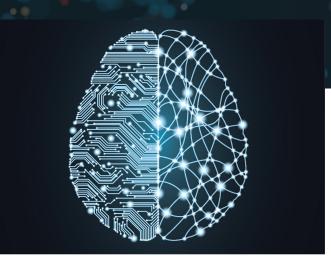# Materials Informatics Expertise

Use Cases

Property Prediction, Materials Discovery, Formulation Optimization, Structure Generation, Materials Compatibility, Materials Safety, Surrogate Modeling, Text Data Mining, Data Management, Data Augmentation, Automated Data Analysis, Literature and Patent Search

Materials

Polymer Compounds, Catalysts for Carbon Utilization, OLEDs, Solid Electrolytes, Polymer Electrolyte Fuel Cell Electrodes, High-entropy Alloys, Engineering Plastics, Synthetic Rubber, Photoresist, Insulating Films, Anisotropic Conducting Films, Lubricants, Photovoltaics, Color Filters, Perovskite Ceramics

Technology Areas

Large Language Models (LLMs), Graph Neural Networks, Bayesian Optimization, Deep Learning, Generative Adversarial Networks (GANs), Natural Language Processing (NLP), Open Data, MD, DFT, Multi-scale Modeling, Electrochemical Simulation, Mathematical Modeling, Molecular Representation, Cloud, Databases, Data Pipelines, Data Ops, ML Ops, Web and Desktop UIs

Enthought is a global leader in scientific computing and materials informatics. We have been developing AI and ML-driven solutions for innovative companies for over 20 years.

Digital Capability Building

Enthought's unique **Materials Informatics Acceleration Program** helps innovation-driven companies build the digital capabilities of their scientists while tackling real in-house problems and creating value-generating software solutions. Our world class team of training and MI experts work alongside and guide scientists to leverage the wealth of tools in the scientific computing ecosystem.

Participants finish the MI Acceleration Program equipped to build data-driven decision support tools using AI and machine learning to accelerate R&D innovation.

Learn more about the Material Informatics Acceleration Program for scientists.

Contact us at info@enthought.com to setup a free 30 minute consultation or demo.