CITRINE INFORMATICS

EBook

DIGITAL TRANSFORMATION AND MATERIALS INFORMATICS

Digital Transformation and Materials Informatics

Industry is going through a digital transformation powered by the enormous technological potential now available - cheap computing power, better database infrastructures, widespread data collection, and powerful AI. Materials and Chemicals companies are not immune to this trend. AccelorMittal, currently the top ranked producer of steel in the world by volume, has as part of its strategy: "Global R&D is focusing on launching digital transformation projects throughout all aspects and segments of the business." In this paper we summarize 4 critical success factors that large materials and chemicals companies have identified in this area and how Citrine's technology fits in to this picture.

Digitalization is a Key Business Initiative for Most Materials and Chemicals Companies

AccelorMittal	Mitsubishi Chemical	Nippon Steel
"Global R&D is focusing on launching digital transformation projects throughout all aspects and segments of the business."	"Promote Digital R&D, such as materials design through full-scale utilization of materials informatics as well as open innovation, and improve R&D efficiency utilizing quantum computing."	"Promoting DX Strategies"
ARCELORMITTAL.com	MITSUBISHI.com	NIPPON.com

Critical success factors for digitalization in materials and chemicals:

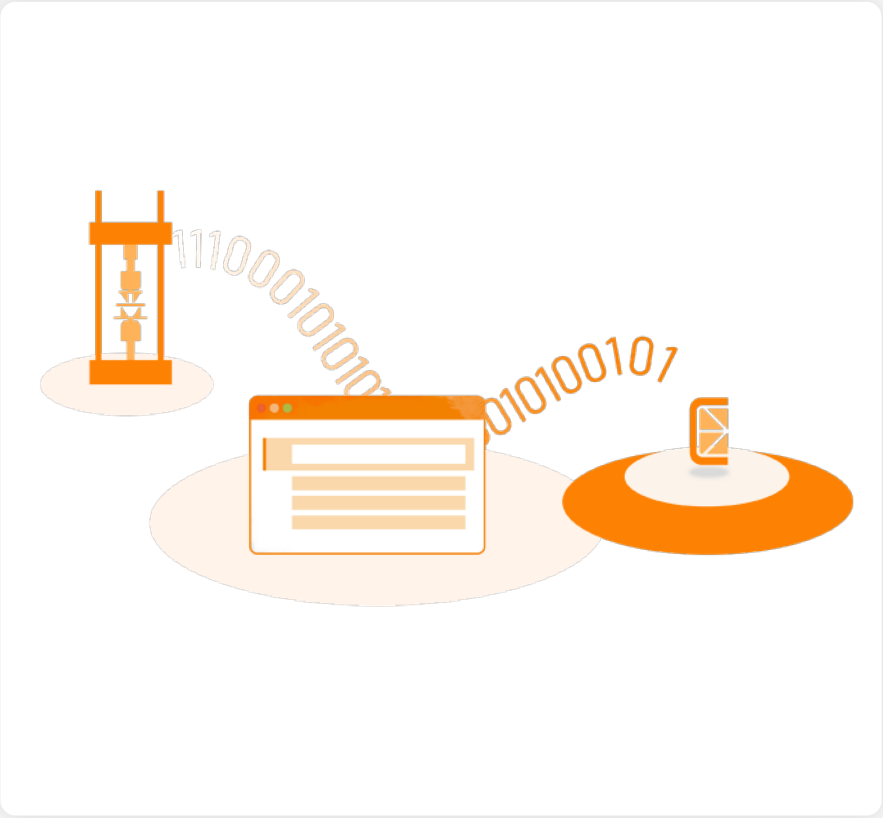
1. BETTER USE OF DATA
2. INTEGRATING DIGITAL TECHNOLOGIES INTO HUMAN WORKFLOWS
3. ENHANCED BUSINESS INTELLIGENCE FOR ACCELERATED DECISION MAKING
4. DIGITAL R&D AND SMART FACTORIES

1. Better use of data

Digital transformation starts with data. While lack of structured data shouldn't stop projects from getting started, quick access to consolidated, clean data powers all other aspects of digitalization.

There are 3 aspects to work on to ensure that decision-makers have actionable data when they need it:

1. **Make data input and integration easier**
   Nobody enjoys data entry but making data entry and structuring as simple as possible increases data entry standardization, accuracy, and usability. In turn, this increases the benefits that scientists will reap from data entry and encourages better behavior in the future. A virtuous cycle.
2. **Collect data automatically from multiple sources**
   Setting up data pipelines from test equipment and sensors deliver large amounts of data without human error or intervention.
3. **Ensure the data platform is comprehensive and well-structured**
   A good data model is key to making sure that the data platform can accept data from various sources, structure it, and store it in a way that future users can use it.

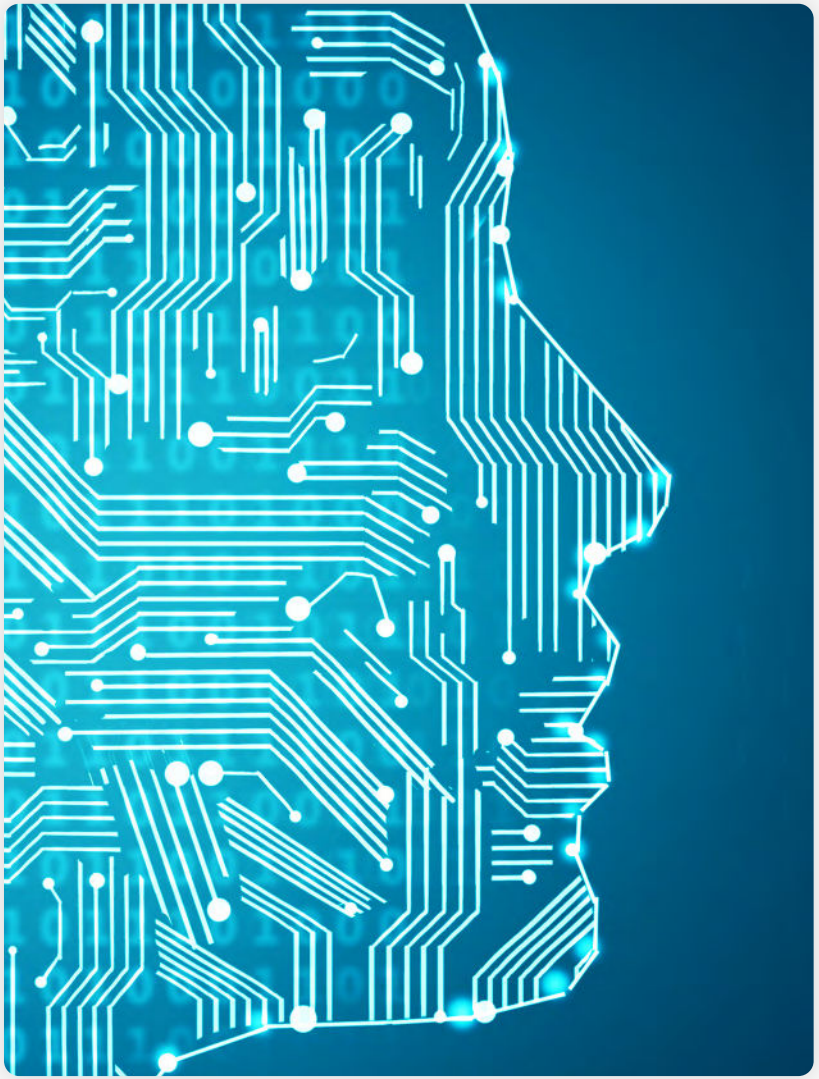


2. Integrating digital technologies into human workflows

The benefits of digitalization can't be realized without conquering the human aspects. While not everybody needs to be a data scientist, many people across an organization need to be comfortable with data-driven methods and adopt new approaches for digitalization to be successful. While the technology needs to be easy to use and deliver value, companies also need to invest in change management, training, and hiring.

There are 3 aspects to consider for successful human/ digital interfaces:

1. **A digital mindset**
   Data-driven decision making needs to be a value ingrained in an organization and modelled by the leadership team. The motivation for acquiring data and the skills to use and visualize it stems from visionary leadership.
2. **Training and hiring for digital skills**
   Research and manufacturing employees usually have the numerical background to thrive in a data-driven environment, but continual professional development opportunities need to be provided to help key staff learn new methods and acquire a common vocabulary. Digital skills need to be incorporated into hiring requirements as appropriate.
3. **Technology to capture and reuse company IP and implicit knowledge**
   Another aspect of the digital-human interface is the use of technology to capture the invaluable but nebulous knowledge that resides in the heads of key employees. By codifying that knowledge, you can make use of it immediately, and have it available for future projects and training new hires.



3. Enhanced business intelligence for accelerated decision making

As more data, and importantly more real-time data, becomes available there are more opportunities for managers to analyze problems, find root causes, and make timely interventions. Decisions previously based on gut-feel and experience, can now be data-driven and shifted earlier in project timelines. Better forecasting and prediction of results mean that positive developments can be capitalized on, and low-likelihood projects shut down or redirected.

There are 3 areas for improvement:

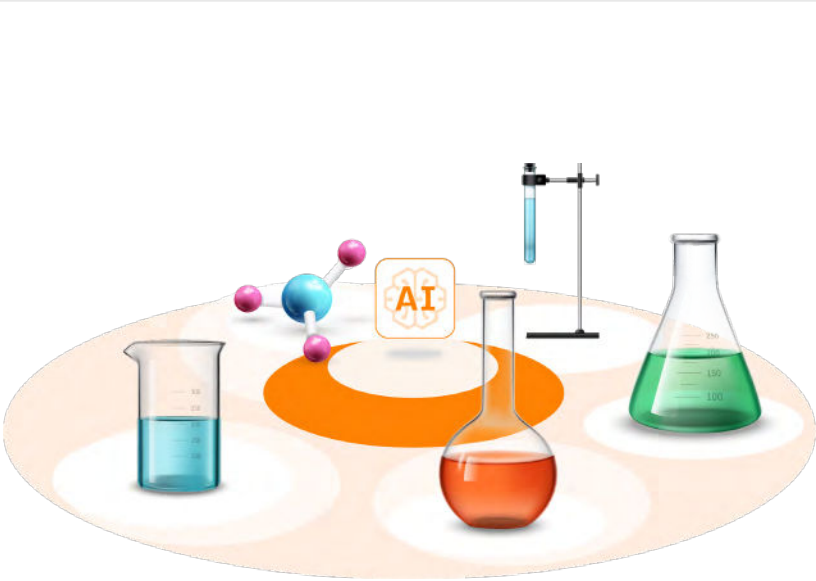
1. **Better analytics for sales and inventory forecasting**
   Structured data and AI enable more factors to be considered for forecasting. Trends can be uncovered that would not have been found with previous methods. .
2. **Gain real-time visibility of key information and KPIs**
   Established data pipelines feed analytics and visualizations that can be refreshed frequently.
3. **Enhanced problem-solving capability**
   Because AI can analyze higher-dimensional, larger datasets than humans, root causes can be easily identified in complex problems.

4. Digital R&D and Smart Factories

Statistical process control has occurred in factories for decades. The use of data-driven decision making here is nothing new; easier collection and analysis of data, and more automation just makes this more powerful. Digital R&D, on the other hand, is more of a culture change. Scientists are used to using lab notebooks and trial-and-error methods honed by their intuition. While some organizations use Design of Experiment methods, this is not universal. R&D is an area where big improvements can be made.

There are 3 Areas Companies are digitalizing:

1. **Agile R&D and Application Engineering**
   AI reduces the number of physical experiments needed to reformulate or discover new materials, leading to quicker R&D timelines. It can also result in expanded recipe banks that can be analyzed against new customer requests. Requests that are more out of the box can be handled by tweaking an existing AI model.
2. **Automated defect recognition, quality assurance, and predictive maintenance**
   Machine vision is used for defect recognition and quality assurance, leading to higher yields. This in turn reduces environmental impacts by using fewer resources. AI can be used to predict when equipment needs to be maintained, reducing downtime and waste.
3. **Integrated logistics and supply chain assurance**
   Getting closer to customers by integrating logistics data systems and offering supply chain transparency enables companies to move to a service-based business model and improve customer relationships.

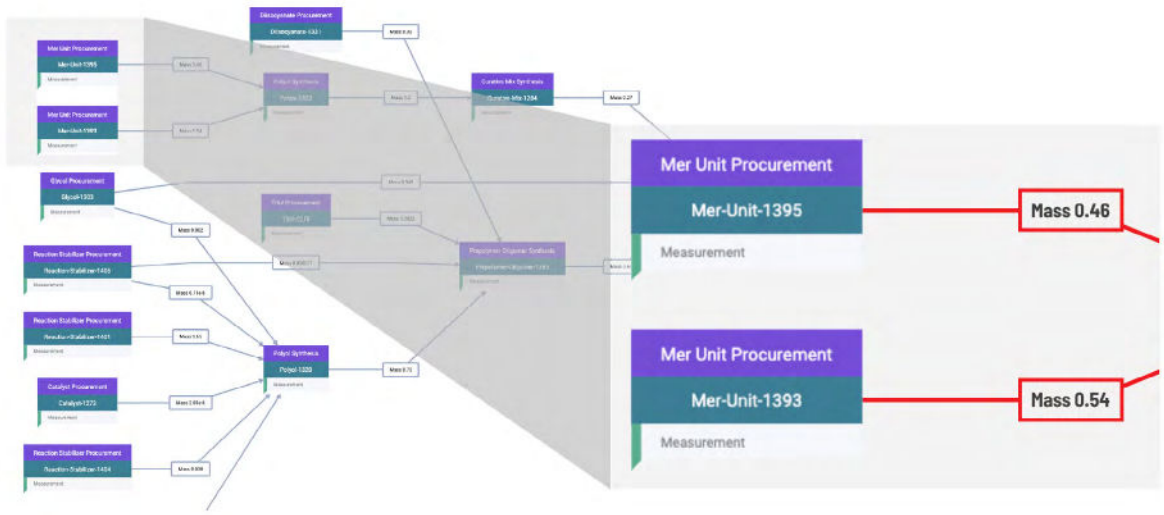


CITRINE'S APPROACH TO DATA MANAGEMENT

Combine your materials and chemicals data from different sources, fill gaps, and make sure it is trusted and accessible

Citrine's unique Graphical Expression of Materials Data (GEMD) data model takes in data from procurement through to characterization and links it together to produce a complete material process history. It then enables interactive and intuitive exploration with links that highlight complex connections. Scientists can retrieve the full context of every data point and data templates can be created to ensure that common properties, measurement techniques, and processing steps are consistent across projects. The ability to find out where data came from and what conditions applied when measurements were taken means that data is trusted and can be reused, reducing repeated experiments. The cloud-based system enables easy access to team members across the globe. Access to datasets and models is controlled via an authorization system within the platform. AI models can be used to fill gaps in data.

Easily explorable material process history

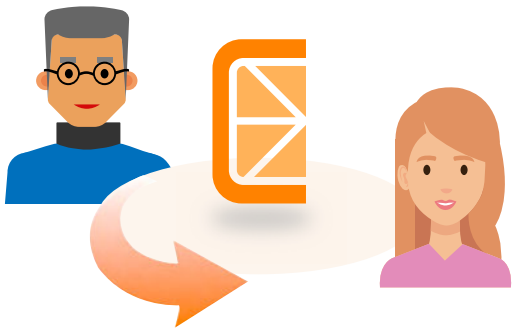


CITRINE'S APPROACH TO DOMAIN KNOWLEDGE INTEGRATION AND SHARING

Integrate domain knowledge (company IP) into AI workflows, preventing the loss of expertise, and accelerating future projects

The Citrine Platform is designed to be interpretable. Graphical AI models can be configured and reused, facilitating collaborative problem-solving between researchers and data scientists. The platform codifies domain knowledge through shareable structured datasets, materials-specific AI models, and scientific feature libraries. The AI models are not a "black box," and a display of feature importance helps researchers see which underlying mechanisms are affecting properties. Future researchers can use these digital assets to accelerate onboarding and project progress.

Integrate domain knowledge



Feature Importance — See all (15)

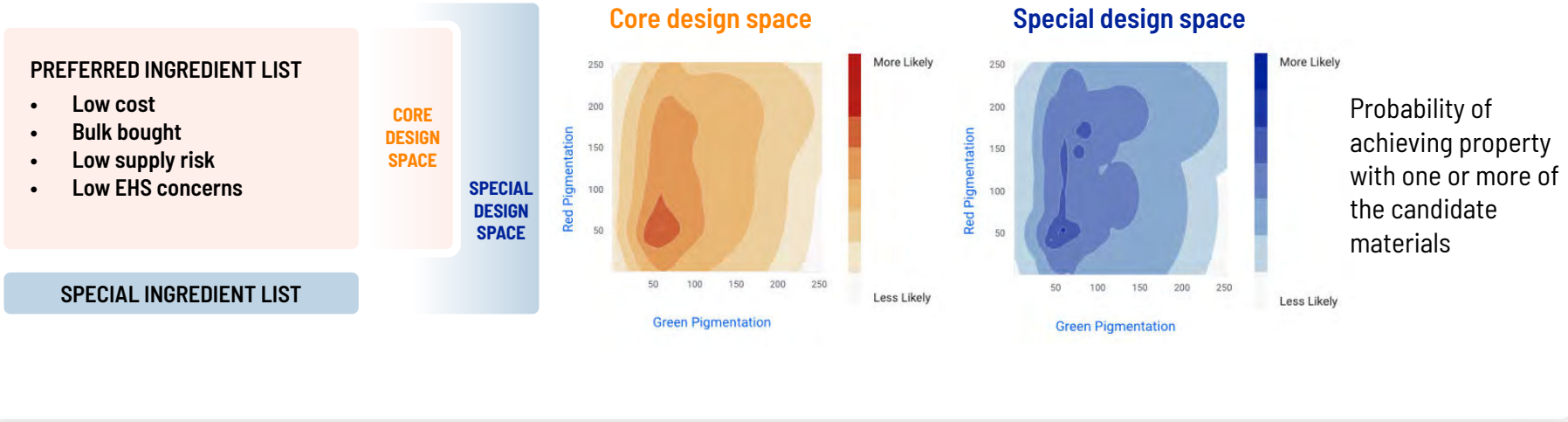
	Name	Importance
1.	Elemental polarizability	0.32
2.	Shear modulus	0.12
3.	Trouton's Ratio	0.10
4.	Ratio of electron affinity to electronegativity	0.07

CITRINE'S APPROACH TO BUSINESS INTELLIGENCE FOR R&D

Quantify the probability of research success and balance project risks

The Citrine Platform's design-space visualization capability calculates uncertainty for each prediction, and patented technology sums the probability of hitting target values across all the candidates in the design space (the matrix of feasible material candidates for the project). The result is a detailed picture of the likelihood that a project direction will achieve the project goals. By changing the design space and running the visualization again, multiple research directions can be compared before entering the lab. Investing additional resources in one research direction has a known risk and opportunity cost. Decision-makers can quickly assess the best route forward.

Compare likelihood of success in different scenarios

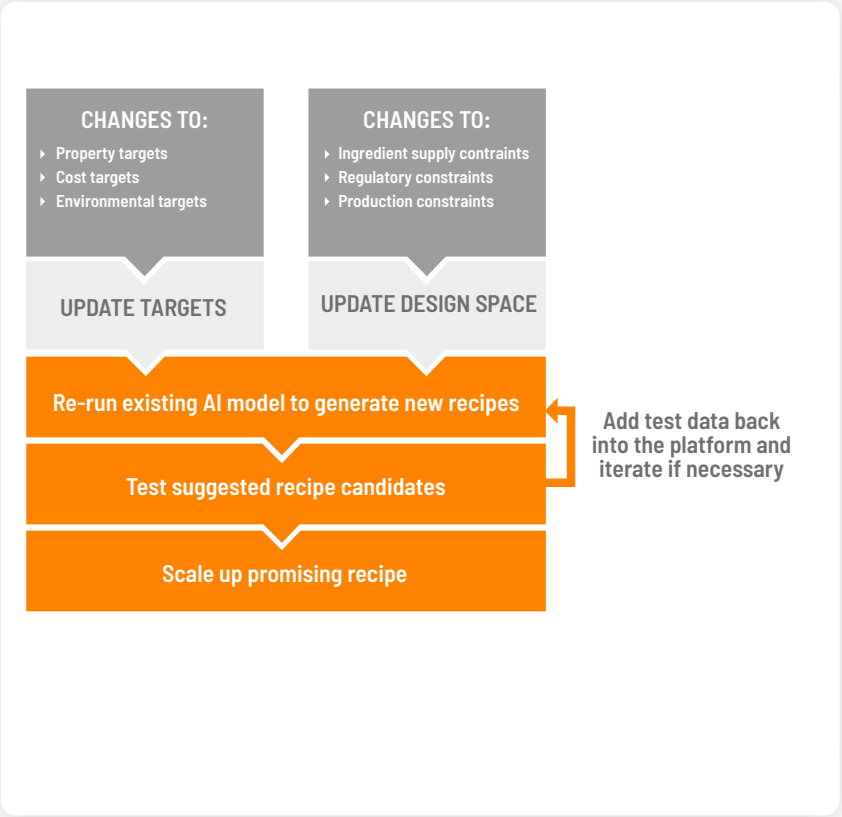


CITRINE'S APPROACH TO AGILE R&D

Make R&D and application engineering more productive and more agile

Rapid change is the new normal, and agility is critical to success. Once AI is embedded in a business unit's workflows, companies respond to new customer performance targets or constraints in weeks rather than months. Updating targets and constraints in an existing project leads to candidate materials in hours. Synthesizing candidates and testing them will still take time, but there's now a higher probability that new candidates will meet or exceed targets.

Projects requiring research in a new area are carried out using a process of AI-guided Sequential Learning, resulting in fewer experiments before the target properties are achieved.[1]



[1] **High-Dimensional Materials and Process Optimization Using Data-Driven Experimental Design with Well-Calibrated Uncertainty Estimates**
Julia Ling, Maxwell Hutchinson, Erin Antono, Sean Paradiso, Bryce Meredig. Integrating Materials and Manufacturing Innovation, 6(3), 207–21 (2017). https://link.springer.com/article/10.1007/s40192-017-0098-z

SUMMARY

Materials Informatics is an important part of any digitalization strategy. Improving data management and exploiting AI produce better results in:

- accelerated R&D
- agile application engineering
- data-driven research decision making
- codifying company expertise in reusable digital assets

Citrine Informatics provides the world-leading materials informatics platform. Founded in 2013, with 85+ employees across 5 countries and 60+ customer engagements, we have the depth of experience needed to help you navigate both the technological and cultural transformation needed to leverage AI and smart data management in the materials and chemicals space. Contact us to find out more.

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