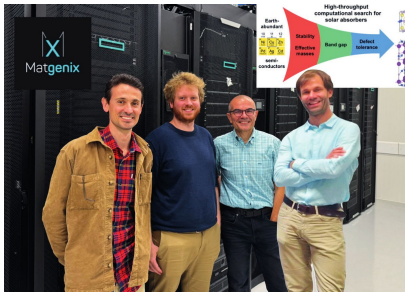
Faced with growing demand from industry for services involving simulations and machine learning, Gian-Marco Rignanese co-founded the start-up Matgenix in 2020 following a First Spin-Off funding from the Walloon Region. It’s a great way of making researchers’ skills available without the usual publication constraints.

## A new era for materials design

The traditional approach for designing materials has long relied on a trial-and-error approach where each step of the process, including synthesis, preparation, testing, and validation, is prone to potential failures. This approach not only consumes a significant amount of time but also incurs high costs, making it inefficient and unsustainable in the long run.

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Recently, a paradigm shift has taken place with the advent of machine learning. Today, the development of materials, compounds, and molecules has reached new heights of speed and optimization. Matgenix leads the charge with a cutting-edge solution built on three core pillars: harnessing the power of artificial intelligence through machine learning, employing advanced data management techniques, and conducting high-throughput computer simulations rooted in real-world experimental data. These pillars seamlessly intertwine through automated workflows, driven by cutting-edge supercomputing technology. Matgenix delivers unmatched efficiency to clients in verifying operations and extracting invaluable data and insights through the deployment of these automation tools across diverse industrial sectors.

## Comprehensive support from idea to commercialization

Matgenix supports its customers throughout the entire innovation process, starting from the idea to the concrete realization, production, and commercialization of their new materials and compounds. It helps its customers to define clear and precise specifications. It proposes tailored work plans matching their business goals and schedule. It identifies the best candidates by executing this work plan and continues to support the implementation and up-scaling of their new materials, compounds, and processes.

## Tailored software solutions

The development of in-house solutions is also part of the Matgenix service offering. The company develops tailored software solutions for its customers' applications: machine-learning models, scientific workflows, automated simulations, etc. It analyzes their needs during its align phase. It then designs the architecture of their solution with high-quality standards and finally, it implements the software into their systems. After the deployment of the software, it provides support and maintenance for using or improving their software.

With this in mind, Matgenix has developed the open-source software turbomoleio in collaboration with BASF. This new tool facilitates the setup and analysis of quantum chemistry computations.

## Early intervention and experimental design

If Matgenix intervenes early enough, it can help its customers with the 'design of experiment' with AI and active learning. For example, Matgenix has developed machine-learning models for Cartier to predict variations in the color of gold and other resulting properties. Matgenix is also active in two Horizon Europe projects.

In NICKEFFECT, it uses active learning and simulation to optimize electrodeposition parameters for Nickel alloys as an alternative to Platinum-group metals. In AEMELIA, Matgenix supports the experimental partners to improve the performance of anion exchange membranes for fuel cells.

## Exploring new frontiers

Other applications are currently being explored: finding new materials-based hydrogen storage solutions for automotive applications using in silico techniques, developing innovative laminated materials for transparent electronics, specialty alloys, chemical and catalytic designs, biomaterials, process optimization, etc. A good way of saving its customers time and enabling them to concentrate on other business ideas.

For the time being, Matgenix's main activity is service-based, but it has not given up hope of developing software that could be marketed. In addition, it has added a new area of work: extended virtual reality with the digital twin and large language models such as ChatGPT. What remains to be determined is the interface that will enable virtual interaction with generative AI.

**Matgenix**
A6K | Advanced Engineering Center
Square des Martyrs, 1- B-6000 Charleroi
Tel. : +32 (0) 479 575 708
Email : info@matgenix.com
https://matgenix.com/