
DAIMON
SIMULATING REALITY
Advanced modelling frameworks
for hi-tech applications

INNOVATION THROUGH MODELLING

Development, implementation and application of modelling and simulation platforms - from large-scale computing to AI for health, advanced manufacturing, energy, environment

DAIMON

ABOUT **US**

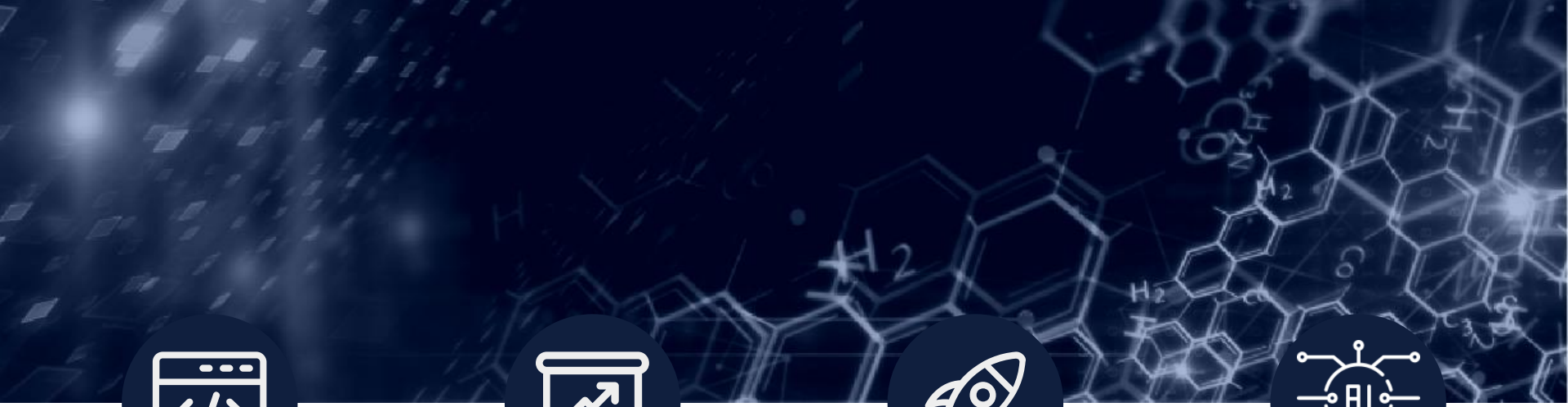
Our activities aim at supporting **research and innovation** strategies for the development, implementation and uptake of **new solutions in industry, research and society** to address global challenges in fields including **health**, **industry**, **energy**, **environment**.

We develop, implement and apply **advanced simulation environments for hi-tech applications**. We believe that digital and virtualization technologies, from **high performance computing** to **artificial intelligence**, can boost innovation in **advanced manufacturing** and **Industry 4.0** or in the development of new systems for **diagnostics** and **therapeutics**.

OUR **APPROACH**

We rely on integrated modelling approaches, including **multiscale simulations**, to assist the design and development of complex systems. Our approach is particularly relevant in applications where properties at a smaller scale impact strongly on the behavior of a system at a macro-scale, as for example in the development of nano/micro **devices**, multifunctional **materials**, and materials **processing**.

The key feature of our approach is **interdisciplinarity**, combining different competences in the definition of new virtualization paradigms, from chemico-physical **modelling** to **data-science**.



Multi-scale modelling

From the properties of **nanoscale materials** to full **devices**, integrating electronic and atomistic **modelling**, molecular dynamics, coarse-grained and continuum-based simulations

Simulations for key technologies

In-silico design, discovery and property prediction applied to **advanced functional materials**, **manufacturing**, **bioelectronics**, **processing**, and others

High-performance computing

Specialized **hardware and software infrastructures**, including access to transnational computing centres, and a large library of **simulation packages**

Machine learning and AI

Application of **big-data** approaches, **deep-learning** and artificial neural networks to extend the predictive capability of modelling and simulations

MULTI-SCALE **SIMULATIONS**

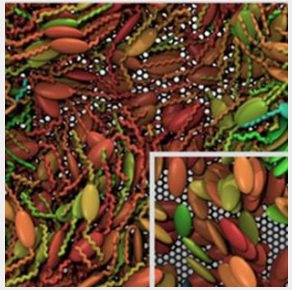
From materials properties to the device scale

- Support to innovation and research by providing multi-scale models of complex systems, integrating **materials properties** into nanoscale, mesoscale, microscale and device-scale features.
- Accurate models of materials properties **across different scales** through **state-of-the-art computational techniques**, from density functional theory calculations to molecular dynamics, coarse-grained simulations and finite-element methods.
- Development and application of **integrated simulation frameworks** based upon chemico-physical criteria, realizing the interconnection across scales. This approach leads to **predictive and efficient tools** for materials modelling, from the design of new materials to processing and use in applications.
- Applications of simulations to understand and develop **innovative platforms in materials science and technology for applications** in fields ranging from energy, health, manufacturing, environment, etc.

DATA-DRIVEN MODELLING **WITH AI**

From ontologies to realistic models

- Merging recent developments of **Artificial Intelligence** with high-level implementations on **high-performance computing** infrastructures.
- Application of **data-driven** technologies to the predictive modelling of materials and devices. **Machine learning** and **neural networks** to develop and predict the properties of novel materials and to optimize processes and devices.
- Development of methods and tools for the **automatic elaboration** of modelling and integrated modelling/experimental data. Representation of the information and knowledge in the applied materials science domain through the **definition and implementation of specialized ontologies.**
- Development of simulation and virtualization frameworks based on **high-throughput and data-driven computational technologies**. Applications of advanced frameworks in several application domains and to technological targets.

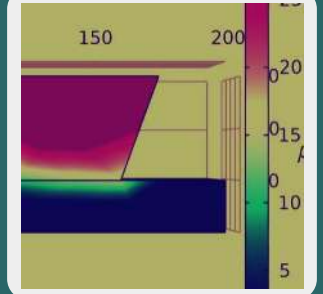


Multiscale materials design

We develop and apply computational models to predict and simulate the properties of materials and interfaces for applications: **molecular materials**, nanomaterials, 2D systems and graphene; macromolecular materials

Materials for life sciences

Understanding the behavior of living matter at the interface with complex systems. Simulations ranging from the atomistic scale to the full device scale enable the development of a wide range of applications, such as biosensors and biomedical devices

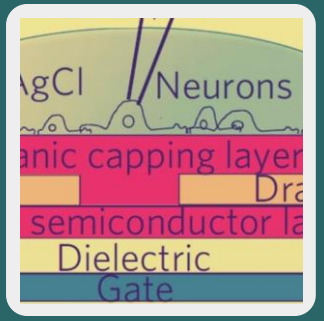


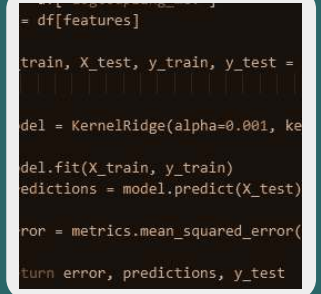
Multiscale modelling of materials processing

We develop and implement multiscale models able to link the molecular properties of materials to their behavior in realistic fabrication setups. Predictive simulations guide the engineering of processing routes for applications

Multiscale modelling of devices

Simulation of multi-functional devices for applications based on advanced materials. Nanoscale electronic devices for **brain interfaces**, electronic and optoelectronic devices (**OLEDs, solar cells**), **sensors**, etc.





Machine Learning and simulation frameworks for materials modelling

We develop integrated modelling frameworks targeted to specific scientific and technological fields. Machine/Deep Learning and HPC enable the realization of high-throughput predictive frameworks

Wide network of collaborations

We participate in **collaborative research projects** and partnerships on HPC and data-driven technologies for the modelling of materials, processes and devices.

Industrial partnerships

Collaboration with industry partners through ad-hoc agreements. Interactions enabled by our connection with **technology transfer** agencies (technopoles, accelerators, incubators).

Administrative flexibility

Formal collaborations with external partners as an **academic** institution, as a **public-private** partnership or as a **private legal entity**, through specific agreements.

Exchanges and visits

Exchange of students, researchers and professionals from academic and private institutions. Support for **visiting and exchange grants** for international fellows and researchers.

DAIMON
SIMULATING REALITY

DAIMON Team - CNR/ISMN
Via P. Gobetti 101, 40129 Bologna, Italy

Francesco Mercuri
Team Coordinator

francesco.mercuri@cnr.it
+39 348 033 2552

www.daimoners.eu
daimoners@gmail.com

Follow us!

twitter.com\Daimoners

Powered by **SensoLato**
www.sensolato.com