

# Section 2: Italian Scientific Cases

## MAX: materials design at the exascale

Materials are crucial to scientific and technological change and industrial competitiveness, as well as to tackle key societal challenges - from energy and the environment to health care, information and communications, industrial processes and manufacturing, safety and transportation. The increasingly high accuracy and predictive power of computer simulations combined with increasingly higher levels of computing power and large amounts of storage capacity of High-Performance Computing (HPC) technologies, now enables a paradigm shift in material design and discovery, in which every increasingly complex material behaviour will be addressed by easily accessible, interdisciplinary, easy-to-use computational experiments.

MaX (Materials design at the eXascale) is a user-driven European Centre of Excellence (ECOE) established to support developers and end-users in materials simulations, design and discovery. MaX focuses in enabling the best use and evolution of HPC technologies by creating an ecosystem of knowledge, capabilities, applications, data workflows, analytic tools and user-oriented services.

At the same time, MaX is enabling the exascale transition in the materials domain, by developing advanced programming models, novel algorithms, domain-specific libraries, in-memory data management, software/hardware co-design and technology-transfer actions.

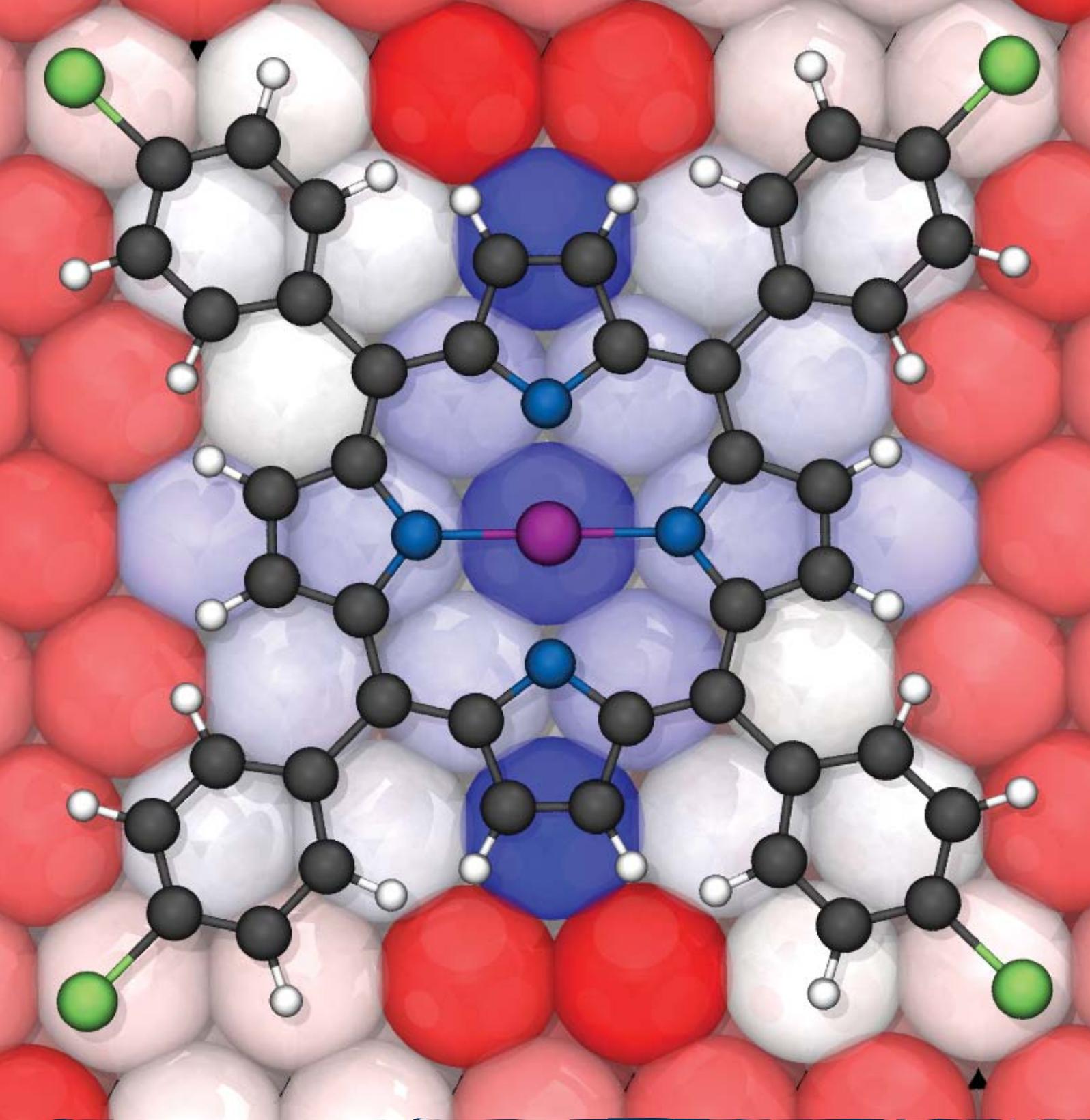
MaX is designed and managed to support the needs and the visions of a number of players:

- **End-users** in research and innovation, both in industry and academia, who explore materials discovery and rely on computer experiments.
- **Domain scientists** who develop new methods, algorithms and tools in materials simulations.
- **Software engineers and vendors** who optimise hardware and software performance and usability together with analytical tools for increasingly efficient computer-assisted materials design.
- **HPC centres and industry** who are interested in empowering the most advanced and ambitious solutions and in hardware-software co-design.

The MaX implementation strategy consists in developing a new application and data ecosystem, and serving its industrial and academic community through end-user oriented actions. MaX key actions include:

- Implementing a **Sustainable Programming Platform** designed to develop quantum engine kernels and low-level domain specific libraries, to facilitate quantum engines' advanced functionalities and to share libraries with other communities/domains.
- Building a **Dynamic Data Framework** to manage the automation of high-throughput calculations, automatic data storage, workflows interchange where data provenance, preservation, reproducibility, and reuse are guaranteed.
- Promoting the **Exascale Transition Enabling Action** through the development of novel algorithms, domain-specific libraries, in-memory data management, and software/hardware co-design.
- Establishing the **User Needs and Solutions Integrating Protocol** by aligning the technological offer with leading end-users requirements.
- Developing a **Catalogue of Services** accommodating end-users help-desk and support, communities' integration, industrial outreach, custom development and consulting.
- Contributing to the diffusion of material simulations by addressing the skills gap through an integrated offer of **Training and Education** programs in HPC and computational material science.

MaX initially focuses on selected flagship codes: widely-used applications, based on rather diverse models, mainly oriented to structural, electronic, magnetic properties and to spectroscopies of materials from first principles: *Quantum Espresso*, *Siesta*, *Fleur*, *Yambo*. A further application, *Aiida*, is the basic informatics infrastructure adopted and developed for workflow and data management, preservation and sharing. MaX will expand the potential of these flagship codes on the present HPC platforms, by implementing new capabilities and algorithms for the study of complex materials, properties and processes in realistic condition, far beyond the current realms. At the same time, MaX will enhance the performance of the flagship codes in terms of scaling,



robustness, and usability, and will make them ready for the forthcoming exascale hardware architectures. In this way, MaX is designing and implementing a sustainable approach of relevance beyond its core codes and field.

MaX will act as a central service hub that will provide project management, coordination and dissemination management for each of the project members, shifting and reducing costs by sharing resources and effort. To guarantee the quality of the provided services MaX will maintain toolsets, templates, and documentation of best practices, procedures, and techniques.

A number of 'Pilot Cases' will be developed in close contact with leading industrial partners representing a challenging test ground for the MaX working approach. The developed packages and work-flows emerging from the Pilot Cases experience will constitute the basis for a 'market-place' where solutions developed for a given problem will be made available and tailored to other end-users. This opportunity is expected to enable rapid response to shorter-term issues, and could be typically well suited e.g. for SMEs.

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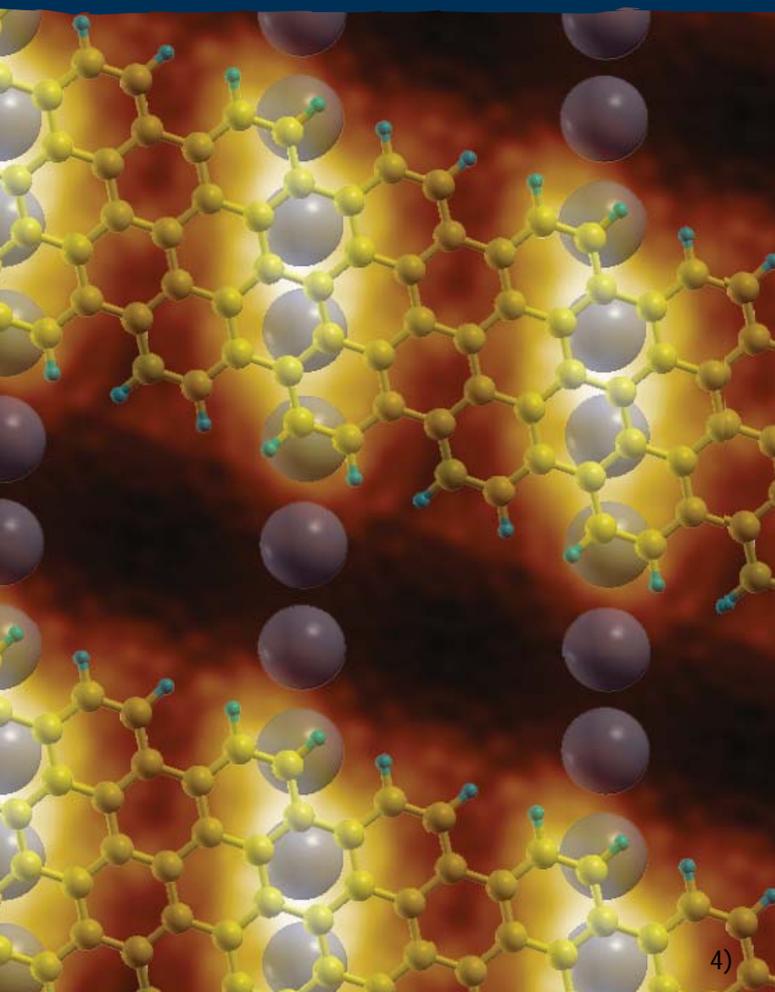
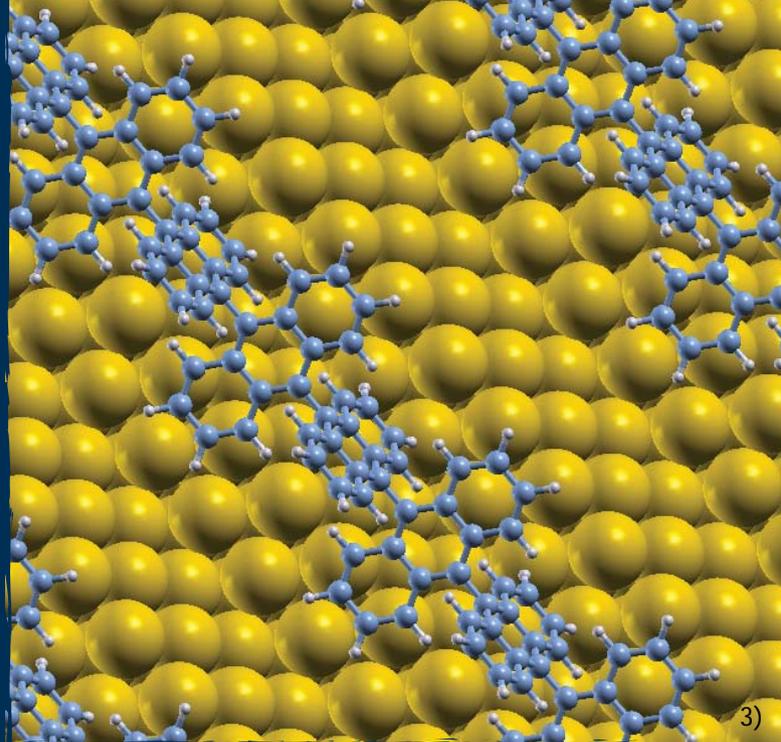
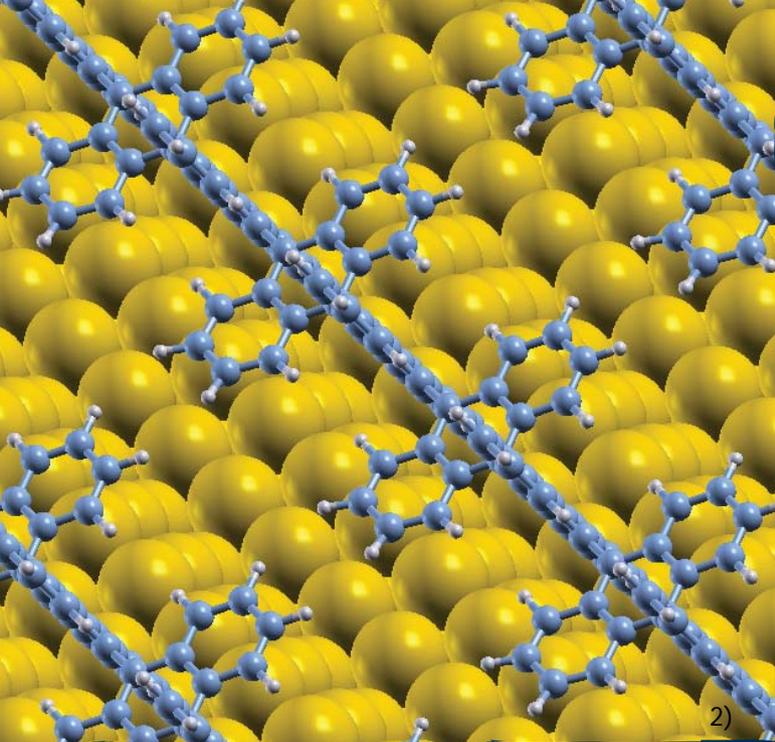
The MaX logo and payoff. MaX communication strategy is aimed at developing a unified and coherent MaX image to enhance community identity among stakeholders. MaX communication style is simple, direct, clear and geometrical. It makes extensive use of basic geometric shapes and of the *less is more* concept in communicating, teaching, and programming.

MaX partners include 5 research institutions: CNR Modena, SISSA Trieste, ICN2 Barcelona, FZ Jülich, EPFL Lausanne. 5 supercomputing centres: CINECA Bologna, ETH/CSCS Zürich/ Lugano, FZ Jülich, KTH Stockholm, BSC Barcelona. 1 global research & education institution: ICTP Trieste. 2 SME business partners in hw and open source technologies: E4 Computer Engineering Scandiano (Reggio Emilia), CloudWeavers London.

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[www.max-center.eu](http://www.max-center.eu)



Graphene Nanoribbon Synthesis on Gold (110) Reconstructed Surfaces.  
 Courtesy of A. Ferretti.

- 1)  
DBBA Precursor
- 2 - 3)  
Polyanthryl formation
- 4)  
Simulated STM image

