



# MAX DRIVING THE EXASCALE TRANSITION



The revolution of the exascale computing ( $10^{18}$  operations per second) is disrupting the capability of computer simulations and data processing. It will have consequences in all scientific fields, including **materials science** as a clear-cut use case.


The road towards exascale technology sets a large number of challenges. **Software:** new development models. **Hardware:** new architectures and the overcome of miniaturisation limits. **Environment:** power consumption of computers (energy to solution) and support of new computing technologies.


## MAX - Materials Design at the eXascale

MAX is a European Centre of Excellence which enables materials modelling, simulations, discovery and design at the frontiers of the current **High Performance Computing (HPC)**, promoting the use of exascale and post-exascale computing capabilities.

MAX challenge lies in redesigning the most used **open source codes** in quantum **materials simulations** and the related data ecosystem in order to take advantage of the exascale technology.

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

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 MaX Centre eXascale

## Join the MAX community!


# MAX DRIVING THE EXASCALE TRANSITION

MAX is proudly co-financed by the European Union for the 2023-2026 period. This Centre of Excellence has received funding for the third consecutive time, a testament to the exceptional expertise accumulated from its prior iterations.


IMPACTS




Bring the most broadly used **open-source codes for quantum simulations in materials to the exascale** by turning them into applications ready to run on HPC exascale platforms. Codes will be ported and scaled on multiple new and heterogeneous computing architectures and optimised in terms of energy efficiency.



**Co-design and energy efficiency with special attention paid to technologies from and relevant to the EU-HPC ecosystem:** Ensure a crossfeed of information and expertise between software and HPC hardware developers to guarantee that new software adapts to future computer architectures and, conversely, new powerful hardware meets the needs of materials scientists.



Foster through MAX's comprehensive training programmes the **engagement and know-how of end-users and developer communities** in industry and academia, in close coordination with the HPC ecosystem in Europe. Widen the access to codes, provide workflows and turn-key solutions to empower user communities in materials simulations to address the most pressing exascale and societal challenges.


























Design and deploy exascale workflows and extreme data handling by addressing key select **scientific challenges in the field of materials science.**

MAX CoE is a partnership of European leaders in the materials domain, prominent European HPC centres, technology partners and training & communication experts.

## EUROPEAN CENTRE OF EXCELLENCE FOR MATERIALS DESIGN

NETWORK

LIGHTHOUSE CODES	DOMAIN EXPERTS & CODE DEVELOPERS	HPC EXPERTS & DATA CENTRES	TECHNOLOGY & CO-DESIGN PARTNERS
    	       	     	   

MAX coordination and management: Cnr – Modena, Italy

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