



DRIVING THE EXASCALE TRANSITION

Materials design at the eXascale - European Centre of Excellence

MaX Principal Goals



Bring the most successful and widely used open-source, community codes in quantum simulations of materials towards exascale and extreme scaling performance



Co-design activities to ensure that future HPC architectures are well suited for materials domain applications and viceversa



Enable the convergence of high-performance and high-throughput computing with high-performance data analytics in the materials domain



Widen the access to codes, provide workflows and turn-key solutions to empower user communities in materials simulations



Foster the engagement and know-how of users communities in industry and academia

Main Impacts

Consolidating leadership in exascale and extreme scale-oriented materials simulation codes

Improved access to computing applications and expertise, leading to scientific discovery and economic and social benefit

Federating capabilities and integrating communities around computational materials science in Europe

A larger number of scientists and engineers trained in the use of computational methods and the development of applications in the materials domain

MaX Partnership



Tier 0
HPC Centres



Codes & ecosystem
developers



Technology
partners



Communication,
training &
dissemination



MaX coordination and management: Cnr - Modena, Italy: management@max-centre.eu

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