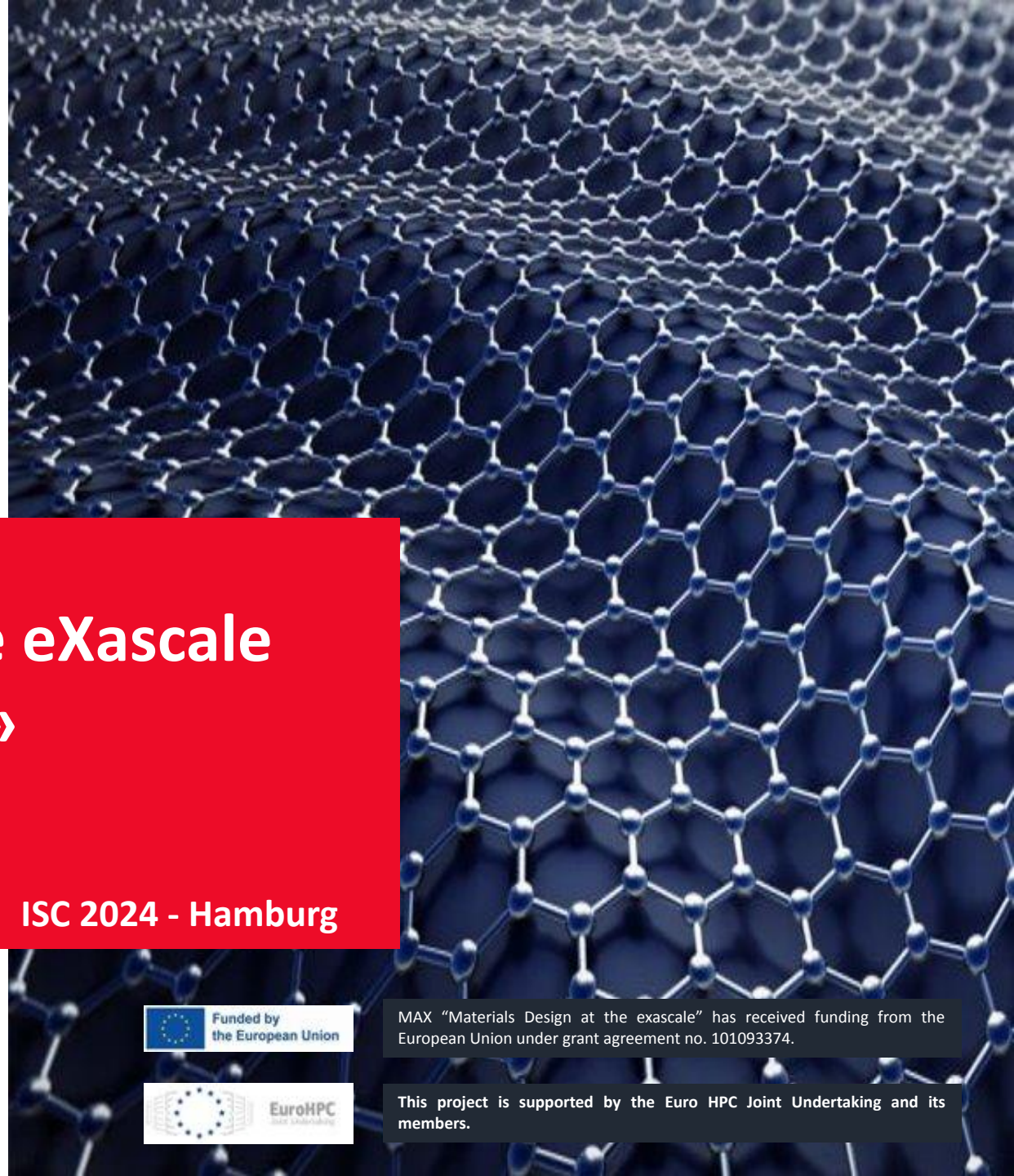
MAX DRIVING THE EXASCALE TRANSITION



MaX – «Materials design at the eXascale European Centre of Excellence»

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EuroHPC

This project is supported by the Euro HPC Joint Undertaking and its members.

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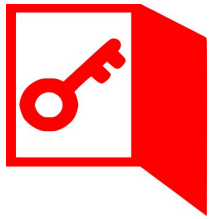
Main Goal

Enable open source community codes in electronic structure (materials science) and their workflows on exascale machines.

4 Key-Actions

1) Restructure MAX flagship codes towards exascale and extreme scaling performance.



2) Design, development and implementation of the architecture and orchestration of the exascale workflows.

3) Co-design and energy efficiency for HPC architectures

4) Widen the access to codes and foster transfer of know-how to user communities.

QUANTUM ESPRESSO

The prime open-source (set of) code(s) for quantum materials modelling using the planewave pseudopotential method.

siesta

A density-functional code able to perform efficient electronic structure calculations and ab initio molecular dynamics simulations of molecules and solids.

Yambo

A code that implements ground-state as well as excited-state properties in an ab initio context.

fleur

A code family for calculating groundstate as well as excited-state properties of solids within the context of density functional theory.

BigDFT

An electronic structure pseudopotential code that employs Daubechies wavelets as a computational basis, designed for usage on massively parallel architectures.

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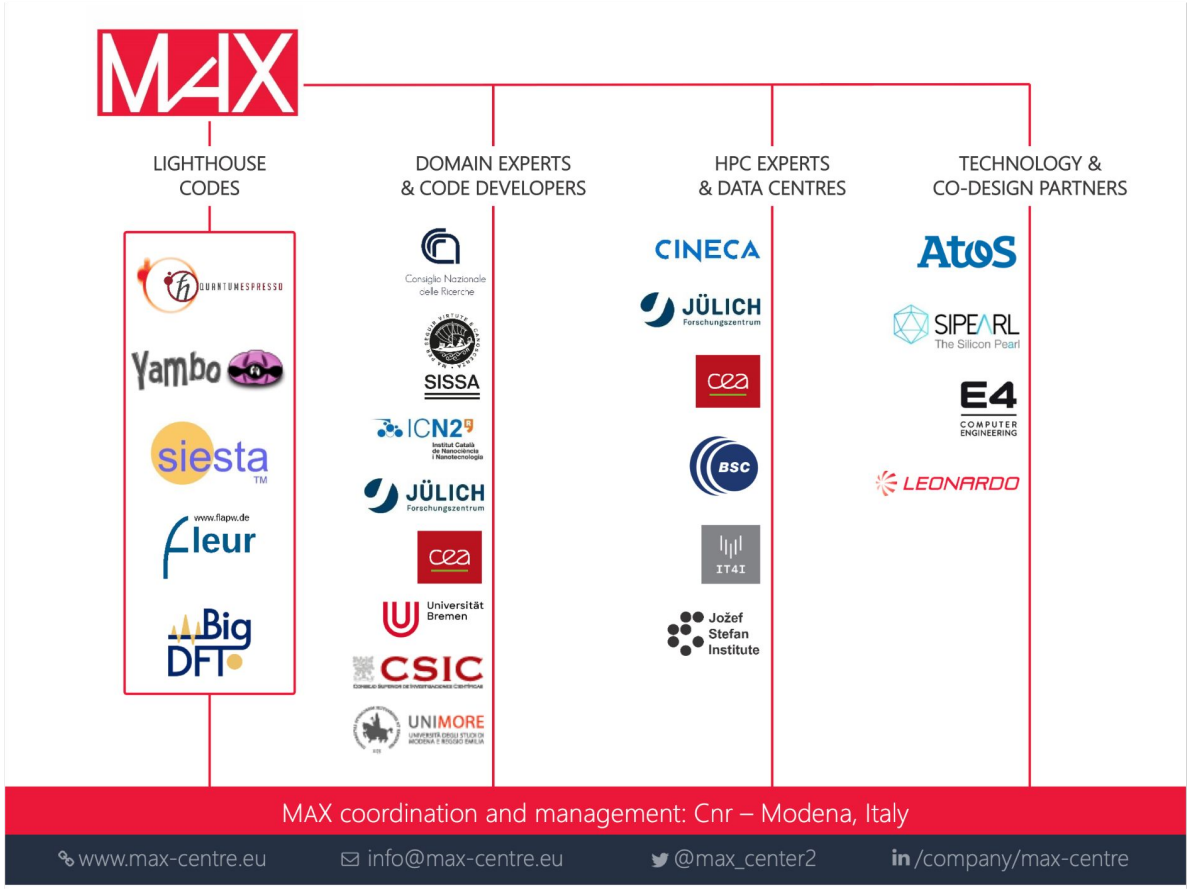

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