Supporting material science at Exascale with MAX Centre of Excellence

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Computational nanotechnology is a branch of nanotechnology concerned with the development and use of computer-based models for understanding, analyzing and predicting the behavior or properties of systems relevant to nanotechnology.
Computational approach has the great advantage of getting informations of the physical/chemical properties of nanomaterials that cannot be investigated experimentally.
Improved methods of modeling and simulation are required to achieve a more robust quantitative understanding of matter at the nanoscale level.

Within MaX Centre of Exellence we support the users for the most advanced applications in the field of nanomaterials based on rather diverse models, mainly oriented to structural, electronic, magnetic properties and to spectroscopies of materials from first principles.
In the background of the Exascale target, a critical aspect of codes used for nanomaterials is their scalablity over a large number of nodes and their implementation of parallel paradigms.
Here we will briefly review the most important codes supported inside MaX with particular attention in the code features as well as parallelizzation aspects and scalability.