Material Science
Materials with specific characteristics are crucial for many industrial products. They can, for instance, improve the performance of existing products or enable entirely new ones. This is achieved through the use of advanced materials science, which is based on an understanding of the fundamental properties of materials.

The material science team at BSC concentrates on numerical simulations for the characterization of new materials. To this end, they develop and implement new approaches and algorithms focusing on both the static and dynamic properties of materials. On the one hand, they conduct the numerical simulations, and on the other hand, they perform simulations aimed at the discovery of new materials.

Objectives

Our research group focuses on numerical simulations for material science research, with the two main research lines “ab-initio electronic structure” and “electronic transport”. In particular, our goals are:

- Development and implementation of new approaches and algorithms for material science research, focusing on atomistic models of solids
- Numerical simulations to discover and characterize new materials. To this end, we use the codes that we develop on our own, but also use external software

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