Material Science
Materials with specific characteristics are crucial for many industrial products. They can, for instance, improve the performance of electronic devices. Furthermore, they may also help to develop new types of materials for future applications, comprising elements of various areas of science such as physics, chemistry, biology, or engineering.

The material science team at BSC concentrates on numerical simulations for the characterization of new materials. To this end, they conduct the numerical simulations, and on the other hand, perform simulations aiming 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 simulations.
- Experimentation and simulation of electronic transport properties in new materials.
- Various collaborations with other research groups.

During the last years, we have various collaborations with other research groups. The main codes which are developed at BSC are SIESTA and BigDFT.

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