Materials with specific characteristics are crucial for many industrial products. They can, for instance, improve the mechanical properties of metal parts, the electrical conductivity of semiconductors, or the biocompatibility of medical implants. The field of material science has become multidisciplinary, 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 performs 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 modeling.
- 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.

We have various collaborations with other research groups. The main codes which are developed at BSC are SIESTA and BigDFT.

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