Material Science
Materials with specific characteristics are crucial for many industrial products. They can, for instance, improve the performance of electronic devices, as in the case of materials used in lithium-ion batteries.

The material science team at BSC concentrates on numerical simulations for the characterization of new materials. To this end, the team conducts both simulations for the characterization of existing materials and on 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.
- 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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