Materials Science
Materials with specific characteristics are crucial for many technological and industrial products. They can, for instance, be used in the field of electronic devices, which requires high performance materials.

The material science team at BSC concentrates on numerical simulations for the characterization of new materials. To this end, they perform simulations using both in-house and externally developed codes. The research group focuses on numerical simulations for material science research, with the two main research lines "ab-initio electronic structure" and "electronic transport". 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, using both in-house and externally developed codes.

Barcelona Supercomputing Center - Centro Nacional de Supercomputación

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