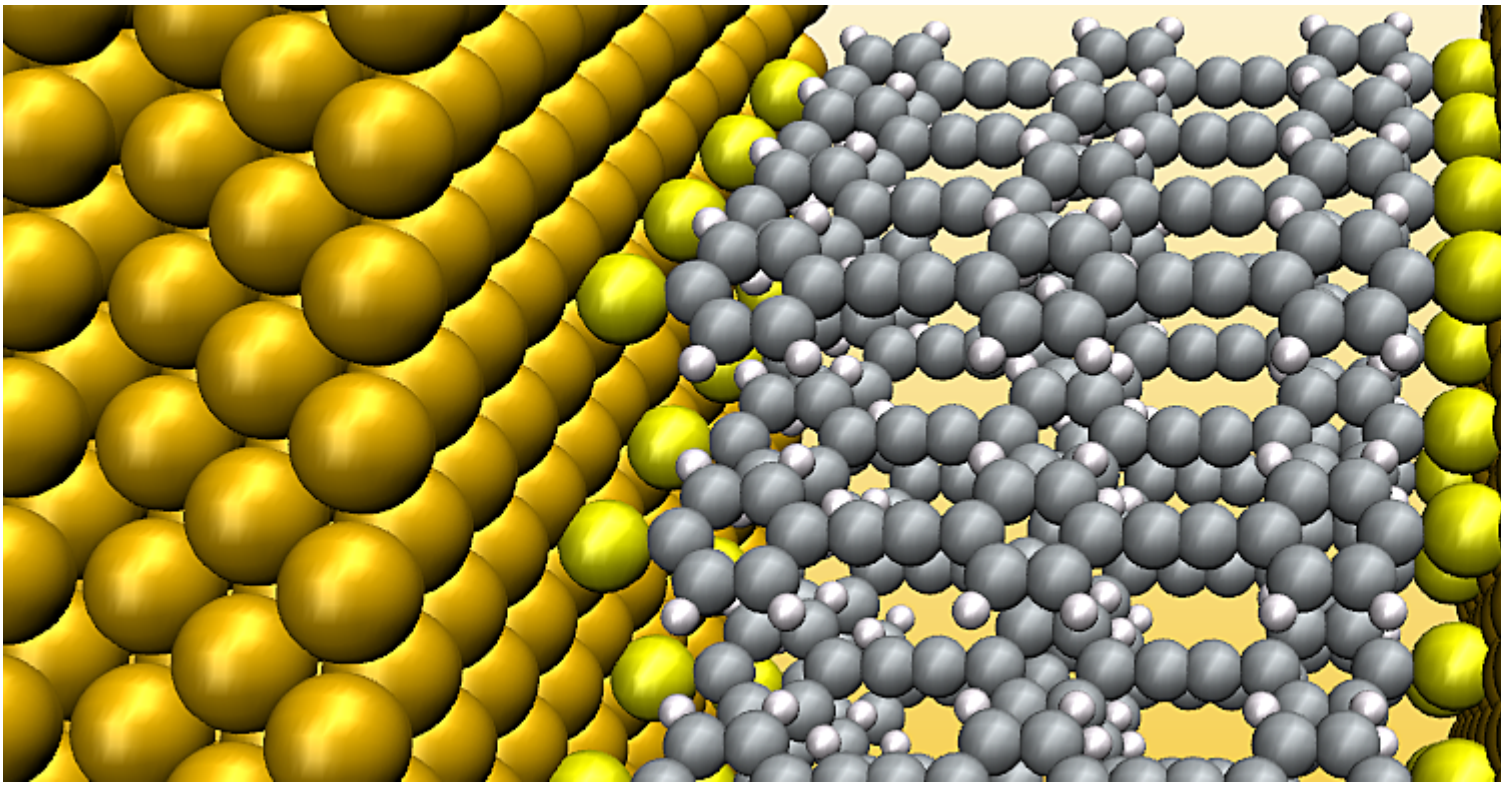
Electronic transport



This research line aims at the development and application of electronic transport simulation tools. We use ab-initio approaches based on fundamental quantum mechanical principles in order to get highly precise and reliable results.

Summary

We are investigating the electronic transport properties of materials, which is a key factor for many applications. We focus on an atomistic description and employ first-principles techniques to get precise and unbiased results. Even though such simulations are computationally very demanding, the steadily increasing power of nowadays' supercomputer and the continuous effort in developing highly efficient codes have made it possible to study systems of realistic sizes and thus to provide valuable insight into the characteristics of these materials.
BSC contributes with HPC related code development as well as assistance with research on tools of various levels of theory. The main contribution is the development of TranSIESTA, a first principles electronic transport simulation tools based on non-equilibrium Greens functions (NEGF). In collaboration with ICN2 also tight binding model based tools are supported.

Objectives

- Improving scalability and performance of simulation tools
- Assistance with execution of demanding simulations
- Representation of simulation tools in large projects
- Collaborate in specific research topics

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