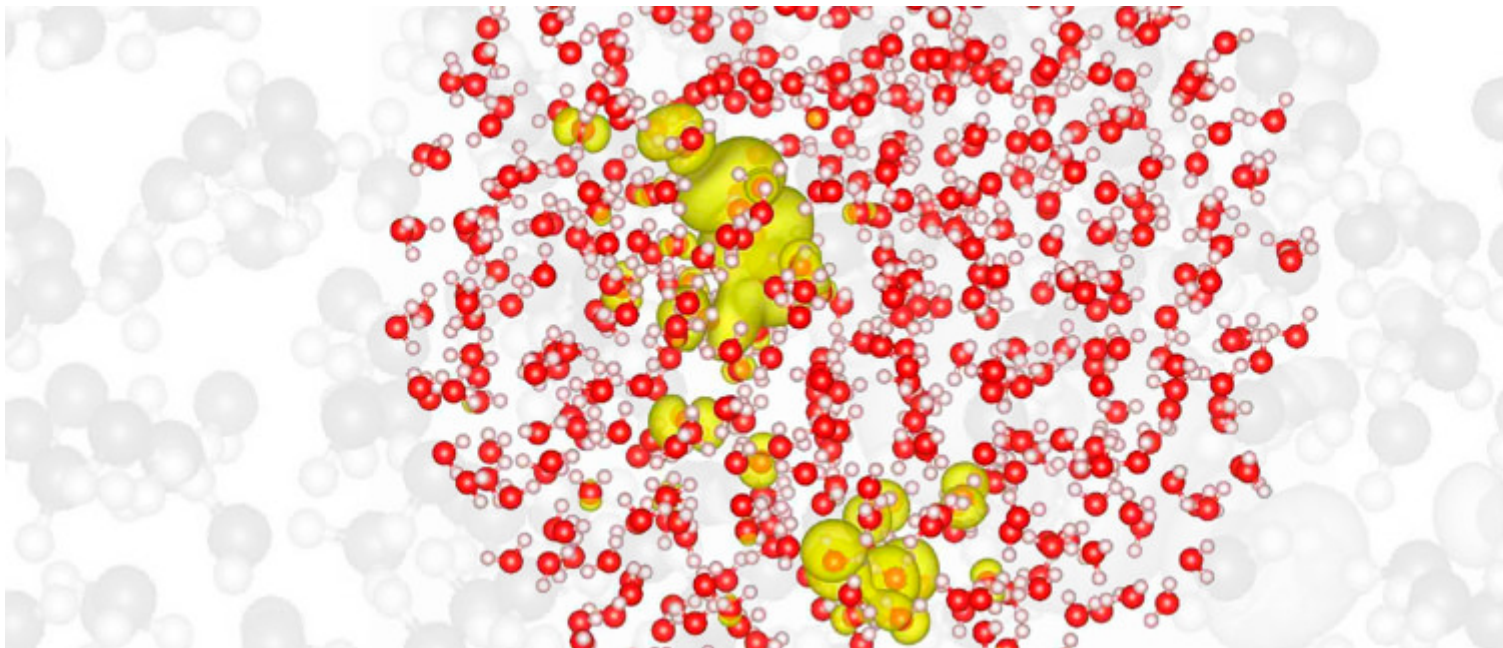


## Ab-Initio Electronic Structure Methods



This research line aims at the development, implementation and application of ab-initio electronic structure methods. These are based on the fundamental laws of quantum mechanics and thus yield a much higher precision than empirical methods. A strong focus lies on linear scaling approaches for large systems.

### **Summary**

Ab-initio electronic structure methods are based on the fundamental laws of quantum mechanics. Unlike empirical approaches they thus do not require any parametrization and consequently exhibit a higher precision, reliability and transferability. On the other hand such first-principles calculation are computationally very demanding and can -- depending on the chosen level of theory -- only handle up to some tens or maybe hundreds atoms.

However, with the constantly increasing power of nowadays supercomputers ab-initio electronic structure calculations become feasible for larger and more complex systems, and ab-initio calculations are now applied in many branches of science, such as physics, chemistry, or material science. The goal of this research line is to work on the development and implementation of such methods, with a strong focus on linear scaling algorithms which allow to considerably increase the system size than can be handled. In addition we perform applications of ab-initio electronic structure methods in various fields, also going beyond the area of material science.

The codes that we are actively developing are BigDFT and SIESTA; however we also use other software

tools in order to perform our simulations.

## Objectives

- Development and implementation of ab-initio electronic structure methods, with a strong focus on linear scaling algorithms
- Characterization and determination of new materials
- Large scale ab-initio calculations

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