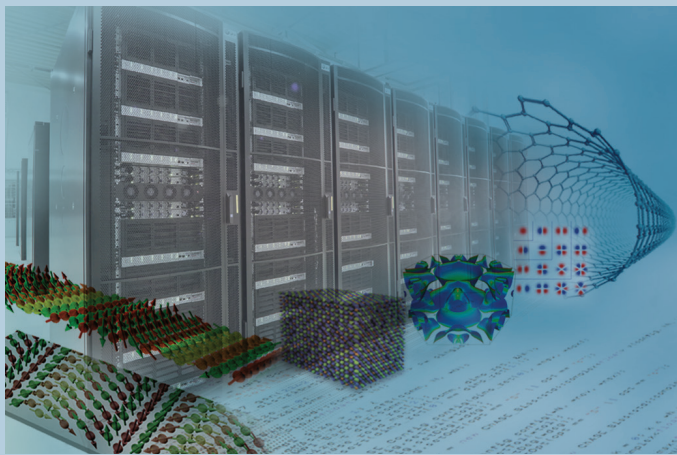


# Simulation Laboratory Quantum Materials

Computational Materials Science on HPC Systems



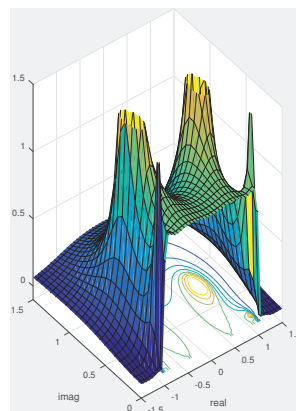
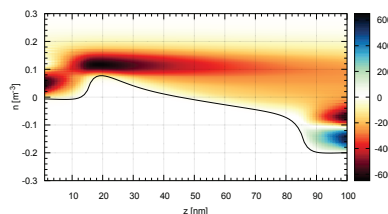
## Mission

The SimLab Quantum Materials:

- Offers expertise in the field of quantum-based simulations in Materials Science
- Provides a high-level support structure in dedicated projects
- Hosts research projects dealing with fundamental aspects of code development, algorithmic optimization, and performance improvement
- Acts as an enabler of large-scale simulations on massive parallel platforms with special focus on high-performance computing

## Research & Support

- Development of Numerical Libraries tailored to computational tasks common to most Materials Science codes
- Modernization and optimization of simulation software
- Foundation of mathematical models and tools for the advancement of computational methods
- Execution and analysis of large scale simulations
- Supporting flexible and sustainable programming practices
- Organization of workshops, symposia, and courses on HPC in Materials Science



## Joint Projects

- Robust methods for achieving self-consistency in large scale DFT simulations (*with FZJ-PG1-1*)
- Inverse design of functional hetero-interfaces in photovoltaic applications (*with FZJ-IEK-5 and RWTH-AICES*)
- Optimized solver for sequences of sparse eigenvalue problems (*with RWTH-AICES*)
- Applying Machine Learning methods to retrieve enthalpies of formation for  $\text{LnPO}_4$  (*with FZJ-IEK-6*)

## Software

- ChASE (*Chebyshev Accelerated Subspace Eigensolver*)
- PAID (*Parallel Adaptive Integration in two Dimensions*)
- KKRnano (*Green's functions Density Functional Theory*)
- FLEUR (*LAPW Density Functional Theory*)
- JuRS (*Real-Space Density Functional Theory*)
- PVnegf (*Non-equilibrium Green's function for PV materials*)

## Know-How

- HPC algebraic eigensolvers
- Pre-conditioners for Density Functional Theory
- Performance Portability
- Algorithm Optimization
- Code Parallelization

## International collaborations

- RWTH Aachen University
- University of Urbana-Champaign
- Oak Ridge National Laboratory
- University of Tsukuba
- RIKEN, AICS
- University of Minneapolis