VSR Seminar

Topic: KKRnano: All-electron density-functional calculations for nanoscale systems

Speaker: Dr. Rudolf Zeller, IAS-3

Contents: In 1929, Paul Dirac made his famous statement that the quantum mechanical equations describe "a large part of physics and the whole of chemistry", but that these equations are "much too complicated to be soluble" and that "approximate practical methods should be developed" which can be used "without too much computation". Here, the Hohenberg-Kohn-Sham density-functional theory (DFT) with an approximate description of electronic exchange and correlation effects represents an enormously successful method (with now more than 15000 publications per year). Nevertheless, the computations are heavy so that systems with more than a thousand atoms can only be treated on supercomputers.

In my talk I will show how KKRnano, our newly developed computer code based on the Korringa-Kohn-Rostoker Green-function method, can be used for this purpose. I will explain the differences with respect to the original KKR method and the techniques which we apply to obtain massive parallelization and to achieve computing times which increase only linearly with the number of atoms in systems, thus avoiding the computational bottleneck of standard DFT calculations where the effort increases cubically. I will show that systems with 100000 atoms (with length scales of about ten nanometers) can be calculated on JUQUEEN and that more than a million parallel processes can be applied for this purpose. I will present applications to GaN doped with Gd (a dilute magnetic semiconductor), GeSbTe (a phase-change material), NiTi (a shape-memory alloy), SrTiO3 (a prototype material for resistive random access memory cells) and for Si doped with P (a prototype material discussed as a quantum computer on a solid-state basis).

Time: Wednesday, 29 October 2014, 14:00

Venue: Jülich Supercomputing Centre, Besprechungsraum 1, building 16.3, room 107

Anyone interested is cordially invited to participate in this event.

sgd Dr. Sabine Höfler-Thierfeldt