

VSR Seminar

Topic: **Exploring the stabilization and manipulation of electronic spins in solids by density functional theory**

Speaker: Dr. Gustav Bihlmayer, IAS-1

Contents: The orientation of individual spins in a solid is determined by relativistic effects, on atomic scale most prominently by the spin-orbit interaction (SOI). In magnetic systems, this is manifested by the magnetocrystalline anisotropy energy and the Dzyaloshinskii-Moriya interaction: both can lead to stable magnetic structures. But even in non-magnetic materials the SOI can couple the electron's spin to its propagation direction, typically at the boundary of a material where inversion symmetry is broken, where it can lead to the Rashba-type spin-splittings. Most prominently, SOI effects arise in two- or three-dimensional materials, known as topological insulators. There, spin-orbit effects in the bulk lead to spin-currents at the edge of the sample, that are by symmetry protected against scattering by non-magnetic perturbations. This protection is of topological origin in reciprocal space, similar to the stabilization of magnetic skyrmions in real space. A quantitative analysis of these tiny relativistic effects would be impossible without calculations based on density-functional theory. These require either large unit-cells or a fine sampling of the properties in reciprocal space, often a combination of both, that are impossible without massively parallelized applications and the support by supercomputing facilities.

Topic: **Modeling of the Coupled Terrestrial Hydrologic and Energy Cycles**

Speakers: Prof. Stefan Kollet, IBG-3

Contents: This talk deals with the development and application of integrated simulation platforms for terrestrial systems. These simulation platforms model the coupled water and energy cycles from the subsurface across the land surface into the atmosphere. Theoretical and technical challenges are discussed in representing nonlinear two-way feedbacks of varying strength, which act over a number of space and time scales. Example simulations are presented from regional catchments toward continental domains. It turns out that initializing the simulations constitutes a major computational problem, because of the long-term memory effects of subsurface hydrodynamics that impact the land surface energy balance and atmospheric processes.

Time: Wednesday, 24 April 2013, 13:30 - 15:00

Venue: Jülich Supercomputing Centre, Hörsaal, building 16.3, room 006

Anyone interested is cordially invited to participate in this event.

sgd Dr. Sabine Höfler-Thierfeldt