O 20: Theoretical methods I

Time: Monday 17:45–19:00

O 20.1   Mon 17:45   A 060

Can we replace a metallic support for an ultra-thin insulating film using a perfect conductor model? — •Ivan Scivetti and Mats Persson — Surface Science Research Centre, the University of Liverpool, Liverpool L69 3BX, UK

The study of atoms and molecules deposited on ultra-thin, insulating films supported by metal substrates is an emerging and exciting area of research, in which Density Functional Theory (DFT) could play a key role. In fact, further understanding of these systems could lead to creation and design of novel functionalized nanostructures or molecular devices for electronics, photovoltaics, information storage and processing, catalysis and chemical sensors [1].

However, DFT simulations of these systems are very challenging, since charging plays in many cases an important role [2]. Therefore, there is a need to develop simplified computational schemes.

In this work we assume that the metallic support can be replaced by a perfect conductor model without having to consider the metal electrons explicitly, which would enable us to handle different charge states and reduce the computational time. To this end, we have developed a novel DFT approach, providing appropriate expressions for the total energy and forces. To evaluate the quality and the range of this approximation, we show preliminary results for adsorbates over an insulating film in different charge states.

[1] Mohn, F et. al., Phys. Rev. Letter 105, 266102 (2010).
[2] Jascha Repp, et al., Science 305, 493 (2004).

O 20.2   Mon 18:00   A 060

juRS - Massively Parallel Real-Space DFT Calculations — •Paul Baumeister, Daniel Wortmann, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich Germany

We present a new DFT tool developed in Jülich that combines equidistant real-space grids and the Projector Augmented Wave (PAW) method. The code is explicitly designed for the structural relaxation of systems consisting of several thousand atoms with very flexible boundary conditions. The real-space treatment of wave functions, densities and potentials enable a simple, efficient and strong parallelization with respect to communication and load balancing. Besides the parallel computation of k-points, we employ a domain decomposition to the real-space cell and a parallelization over eigenvalues (bands). Hence, we exploit the local character of the Kohn-Sham equation and approximate the kinetic energy operator with a localized high-order finite difference stencil. The extremely sparse Hamiltonian favours iterative diagonalization schemes. We will discuss the difficulties due the interplay of wave function convergence and density convergence. Further, we will demonstrate the efficiency of the parallelization on massively parallel supercomputer architectures such as IBM's BlueGene which support cartesian nearest neighbor communication on the hardware level.

O 20.3   Mon 18:15   A 060

Implementation of screened hybrid density functionals for periodic systems with numerical atomic orbitals:Basis function fitting and integral screening — •Honghui Shang and Jinlong Yang — University of Science and Technology of China, Hefei, China

In hybrid functional calculations of the electronic structure, evaluation of the Hartree-Fock exchange (HFX) is currently the computational bottleneck. Although the scaling with system size can be linear when numerical atomic orbitals (NAOs) are used, the computation of HFX carries a large prefactor. The development of efficient algorithms that reduce the prefactor therefore becomes crucial. In this work, an efficient $O(N)$ implementation of screened hybrid density functionals is presented for periodic systems. NAOs of valence electrons are fitted with gaussian type orbitals (GTOs), which can be used for an analytical evaluation of the electron repulsion integrals (ERIs) that are the

building blocks of HFX. The strict locality of the NAOs is employed for an efficient two-electron integral screening technique. In this way, the prefactor of HFX is significantly reduced while retaining the $O(N)$ scaling. This hybrid scheme, denoted as NAO2GTO, is implemented in the SIESTA package. We have tested our method for a variety of systems ranging from molecules to solids. When the DZP basis set is used, good agreement with results obtained from plane wave packages is reached. Our implementation, for the first time, enables screened hybrid functional calculations using NAOs for non-trivial periodic systems.
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O 20.4   Mon 18:30   A 060

A linear-scaling DFT+U study of Friedel oscillations and localization in very dilute Gallium Manganese Arsenide — •David D. O'Regan[1,2], Nicholas D. M. Hine[1,3], Mike C. Payne[1], and Arash A. Mostofi[3] — [1]Cavendish Laboratory, University of Cambridge. — [2]Theory and Simulation of Materials, École Polytechnique Fédérale de Lausanne. — [3]The Thomas Young Centre and the Department of Materials, Imperial College London.

We tackle the long-standing difficulties of large system size and strong electronic correlation simultaneously in this work, demonstrating a linear-scaling DFT+U method [1]. Our implementation within the ONETEP code [2] allows for full local orbital optimization and thus systematic variational convergence, and we demonstrate scaling up to 7,000 atoms. Our method furthermore allows for nonorthogonal projectors [3], which may be self-consistently optimized [4].

The ferromagnetic interaction between distant localized magnetic moments in the prototypical dilute magnetic semiconductor (Ga,Mn)As is mediated by defect-induced holes, whose long-ranged character is critical. We present DFT+U calculations of 1,728 atom super-cells of (Ga,Mn)As, accessing the very dilute (0.1%) limit. We analyze the localization and symmetry of the hole density, and characterize its long-range Friedel oscillations.

[1] O'Regan, Hine, Payne and Mostofi, *submit.* (2011), *arXiv*:1111.5943.
[2] Hine et. al. *Comp. Phys. Commun.*, **180**, 1041 (2009).
[3] O'Regan, Payne and Mostofi, *PRB* **83**, 245124 (2011).
[4] O'Regan, Hine, Payne and Mostofi, *PRB* **82**, 081102(R) (2010).

O 20.5   Mon 18:45   A 060

Analysis and elimination of the linearization error within the FLAPW method — •Gregor Michalicek, Markus Betzinger, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The full-potential linearized augmented-plane-wave (FLAPW) method is widely considered to be one of the most accurate electronic structure methods for solids, providing the density functional answer to high precision. Within the atom-centered muffin-tin (MT) spheres, its basis consists of solutions to the radial scalar-relativistic Dirac equation evaluated at a predefined energy parameter and – as is characteristic of linearized methods – also includes their first energy derivatives to allow for variations around the energy parameter. In some cases, however, the flexibility of the basis is insufficient, and the remaining *linearization error* noticeably affects calculated physical quantities, e.g., equilibrium lattice constants and band gaps. Then, the results may also depend on parameters that are not convergence parameters, such as the MT radii and the energy parameters. To remove the dependence and improve the numerical precision, we analyze in detail how the basis can be extended in a systematic manner by adding local orbitals, defined with either energy parameters at higher energies or second-order energy derivatives. Furthermore, improving the MT part of the basis in this way leads to a faster basis-set convergence so that the resulting basis yields a higher precision than the popular APW+lo method at equal basis-set sizes.