SYEC 1: Exact-exchange and hybrid functionals meet quasiparticle energy calculations I

Time: Thursday 9:30–12:30 — Location: A 151

Invited Talk SYEC 1.1 Thu 9:30 A 151
Nonlocal exact exchange: range separation, hybridization, and local variants — •GUSTAVO SCUSERIA — Rice University, Houston, Texas, USA

This presentation will address our current efforts to develop more accurate exchange-correlation forms for density functional theory. There are two leading themes in our current work: range separation and local weights. On the first theme, we will present a three-range hybrid functional and discuss the rationale for the success of screened functionals like HSE and LC-wPBE. On the second theme, the emphasis will be on new metrics for local hybridization and local range separation.

Invited Talk SYEC 1.2 Thu 10:00 A 151
Magnetization-current density-functional theory — •ANDREAS GÖRLING — Lehrstuhl für Theoretische Chemie, Egerlandstr. 3, 91058 Erlangen, Germany

A magnetization current density-functional theory is introduced that represents a framework for a unified treatment of magnetic effects, noncollinear spin, spin-orbit interactions, and currents of the electron density as well as of the magnetization. A corresponding exact-exchange magnetization-current density functional is presented and used in an implementation of the new approach. This implementation employs plane wave basis sets and pseudopotentials that take into account spin-orbit coupling. First results for atoms and molecules are presented.

Refs.: S. Rohra and A. Görling, Phys. Rev. Lett. 97, 013005 (2006). S. Rohra, E. Engel, and A. Görling, submitted; arXiv:cond-mat/0608505.

Invited Talk SYEC 1.3 Thu 10:30 A 151
GW and hybrid functionals applied to extended systems — •GEORG KRESSE — Faculty of Physics, University of Vienna

GW calculations are presented for small gap and large gap systems, comprising typical semiconductors (Si, SiC, GaAs, GaN, ZnO, ZnS, CdS and AlP), insulators (C, BN, MgO, LiF) and noble gas solids (Ar, Ne). The general finding is that single shot G0W0 calculations using wavefunctions obtained by conventional density functional theory calculations yield too small band gaps, whereas G0W0 calculations following hybrid Hartree-Fock density functional calculations tend to overestimate the band gaps. This is at first sight astonishing, since hybrid functionals themselves yield very good band gaps. The contradiction is resolved by showing that the a proper treatment of the attractive electron-hole interaction (excitonic effects) is required to obtain good static and dynamic dielectric functions using hybrid functionals. The corrections are incorporated in GW using vertex corrections, and the inclusion of these vertex corrections rectifies the predicted band gaps.

In order to remove the dependency on the initial wavefunctions, self-consistent GW calculations are presented, again including a many body treatment of vertex corrections. The results are in excellent agreement with experiment, with a few percent deviations for all considered materials. Finally an outlook on total energy calculations based on GW methods is given and the shortcommings of hybrid functionals are discussed in this light.

Invited Talk SYEC 1.4 Thu 11:00 A 151
Electronic properties of solids within a GW-based DFT scheme: Local versus non-local hybrid functionals — •ANGEL RUBIO — European Theoretical Spectroscopy Facility (ETSF), Dpto Fisica de Materiales, Universidad del Pais Vasco, Centro Mixto CSIC-UPV, San Sebastian, Spain

In this talk we will show alternative treating of correlation effects within a density-functional-based approach based on the adiabatic-connection fluctuation-dissipation theorem (ACFDT) and the linearise Sham-Schlüter. In this context we have calculated the RPA energies as well as the structural properties of simple solids (Si, NaCl). As expected, there are minor differences between the KS-LDA and the RPA results. However, in model layered systems, where layer-layer interactions are very weak, there are evident discrepancies due to the presence of long-ranged correlations. We will discuss the implications for the gap and optical properties in a KS and generalised KS formalisms.

Work done in collaboration with M. Gruning, A. Marini and P. Garcia-Gonzalez. References: Advanced Correlation Functionals: Application to Bulk Materials and Localized Systems P. Garcia-González, J.J. Fernandez, A. Marini and A. Rubio, J. Phys. Chem. B , (2007); First-Principle Description of Correlation Effects in Layered Materials; A. Marini, P. García-González and A. Rubio Phys. Rev. Letts 96,); Density functionals from many-body perturbation theory: the bandgap for semiconductors and insulators M. Grüning, A. Marini and A. Rubio J. Chem. Phys. 124, (2006), and Effect of spatial nonlocality on the density functional band gap, Phys. Rev. B 74, (2006)

Invited Talk SYEC 1.5 Thu 11:30 A 151
The Quasiparticle Self-Consistent GW Approximation — •MARK VAN SCHILFGAARDE — Arizona State University, Tempe AZ

In many-body perturbation theory, the self-energy Σ is constructed in a perturbation expansion in some noninteracting quasiparticles, generated by a noninteracting hamiltonian H_0 or Green's function G_0. The perturbation theory generates an interacting Green's function G. We introduce the idea of a self-consistent perturbation, where G_0 is chosen to be as close as possible to G, to minimize the size of the perturbation. We have implemented the idea in the GW approximation, which we call the quasiparticle self-consistent GW (QSGW) approximation. QSGW handles both itinerant and correlated electrons on an equal footing, in a true *ab initio* manner. It describes optical properties in a wide range of materials rather well, including cases where the local-density and LDA-based GW approximations fail qualitatively. Self-consistency dramatically improves agreement with experiment, and is sometimes essential. Weakly correlated materials such as Na, and *sp* semiconductors are described with uniformly high accuracy. QSGW reliably treats many aspects of correlated materials. Spin wave spectra in Fe, MnO, NiO and MnAs are uniformly well described.

QSGW avoids some formal and practical problems encountered in the LDA-based and self-consistent GW, which will be discussed. Discrepancies with experiments are highly systematic and increase with localization of the eigenfunctions. We will present results for several materials classes to illustrate this, and offer arguments to show what extra diagrams must be included to account for the discrepancies.

Invited Talk SYEC 1.6 Thu 12:00 A 151
Ab-initio Many-Body Perturbation Theory of Electrons, Holes, Excitons, and their Dynamics — •MICHAEL ROHLFING — Fachbereich Physik, Universität Osnabrück, Osnabrück, Germany

Excited electrons, holes, and correlated electron-hole pairs are of prime importance for the spectral properties of condensed matter. They are described by many-body perturbation theory (MBPT), which systematically includes electronic exchange-correlation effects. The most common realization of this approach is Hedin's GW approximation to the electron self-energy operator, combined with solving the Dyson equation of quasiparticles (electrons and holes) and the Bethe-Salpeter equation (BSE) of electron-hole pairs. This GW+BSE method has turned into a standard procedure for many systems, from bulk crystals to defects, surfaces, polymers, molecules, and adsorbate systems.

We will present the GW+BSE method and its relation to other approaches and discuss a number of prototypical systems and results. Particular emphasis will be put on the dynamics related to electronic excitations. On the one hand, the excited state on its own may be subject to femtosecond dynamics of the electronic degrees of freedom. On the other hand, the dependence of the total energy on the geometry may be different in the excited state, causing structural relaxation, spectral broadening, and Stokes shifts. In particular, we discuss prototypical excitations at surfaces, like charge-transfer processes at molecules on insulators [CO:MgO(001)] and particle expulsion from insulator surfaces [KI(001)] and semiconductor surfaces [H:Si(001)].