

Albert J.

9:45 a.m. Thursday, April 21, 331 Smith Hall

Moscowitz Memorial Lectureship

Professor

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Many body methods for condensed matter: current status and future developments

Website: <http://cmp.univie.ac.at/>

Abstract

The properties of all materials arise from the quantum mechanics of their constituent electrons under the influence of the field of the nuclei. The solution of the underlying many-electron Schrödinger equation is a non-polynomial hard problem, owing to the interplay of the electron-electron repulsion and the Pauli exclusion principle. The dominant computational method for describing materials has been density functional theory, although this approach involves uncontrolled approximations. Methods based on an explicit ansatz for the many-electron wavefunctions are potentially more accurate and systematically improvable, but they have not been extensively applied to the solid state because of their computational complexity, which ranges from exponential to high-order polynomial in the number of electrons.

This talk will discuss recent breakthroughs in this field covering quantum chemistry methods as well as Green's function based many body perturbation theory. Results for the hierarchy of quantum-chemical techniques ranging from simple perturbational methods, such as Moeller Plesset theory, over coupled cluster techniques, up to configuration interaction quantum Monte Carlo are presented for a variety of solids. As for molecular systems, coupled cluster methods are found to be very accurate for weakly correlated systems, however, the steep increase of the computational cost makes predictions for real materials still very timeconsuming. Simpler methods that recover the important ingredients of the many electron solution, such as the random phase approximation to the correlation energy, as well as improvements to this method are discussed alongside illustrative examples for important materials. The talk will finish with an outlook on the challenges lying on the road towards validated first principles predictions.

The Moscowitz Memorial Lectureship in Chemistry was established by friends and colleagues of Professor Albert J. Moscowitz (1929-1996) to honor his many contributions to molecular spectroscopy. He was known for his research on the interpretation of optical rotation and circular dichroism spectra in terms of the structures of chiral molecules. In collaboration with colleagues in the medical sciences, he developed important applications of his methods to biomedical systems. Throughout his career, Moscowitz held numerous visiting professorships at other universities, and served on the editorial boards of the leading journals in chemical physics. His work was honored by election as Foreign Member of the Danish Royal Academy of Sciences and Letters, and as a Fellow of the American Physical Society.

Past Albert J. Moscowitz lecturers include Bruce Berne, Columbia University (2000), R. Stephen Berry, University of Chicago (1998), Jean-Luc Bredas, University of Arizona (2002), Mike Duncan, University of Georgia (2010), Crim F. Fleming, University of Wisconsin (2006), C. Daniel Frisbie, University of Minnesota (1999), Mike Frisch, Gaussian (2008), Anthony Legon, University of Bristol (2013), Marsha Lester, University of Pennsylvania (2011), Frank Neese, Max-Planck Institute for Chemical Energy Conversion (2014), Stuart Rice, University of Chicago (2000), Peter Rossky, University of Chicago (2006), Giacinto Scoles, University of Princeton (2004), Benjamin Schwartz, University of California, Los Angeles (2007), Hirata So, University of Illinois, Urbana-Champaign (2011), Walter Thiel, Max Plank Institute, Muelhiem (2002), and Zhen-Gang Wang, Cal-Tech (2014).

Professor Georg Kresse was born on July 21, 1967, in Vienna. He completed his thesis at the Institute for Theoretical Physics at the Vienna University of Technology in 1993, under the supervision of Jürgen Hafner. Kresse was then employed as a scientific assistant in Vienna and held a post-doctoral position at Staffordshire University with Mike Gillan. After the habilitation at the Vienna University of Technology in 2001, he was offered a full professorship from Oxford University as well as from the University of Vienna. He accepted the chair for Computational Materials Physics in Vienna in 2007.



Kresse is full member of the Austrian Academy of Sciences since 2011, and of the International Academy of Quantum Molecular Sciences since 2012. He is the recipient of several awards, including the 2003 START Grant of the Austrian Science Fund (FWF), and the Hellmann Preis of the Internationale Arbeitsgemeinschaft für Theoretische Chemie.

His main scientific interests cover theoretical solid state physics, surface sciences and computational materials physics. His work on ab initio density functional theory for solids, liquid and amorphous systems, and surfaces has contributed significantly to both fundamental and applied research and has shaped the use of density functional theory worldwide.

Kresse is the principal author of the VASP (Vienna ab initio simulation package) computer code that his research group continues to develop. Internationally, VASP is the most widely used program for quantum mechanical simulations of condensed matter systems. The publications underlying this code boast more than 20,000 citations each and are amongst the 100 most cited research articles.

Currently, Kresse directs the Special Research Area Vienna Computational Materials Laboratory funded by the Austrian FWF, whose main goal is the highly accurate description of electron correlations in solids. This project will pave the way to the precise prediction of mechanical, electronic and optical properties in condensed matter. He is the author of more than 350 research articles and has an h-index of about 85.

Host: Professor Donald Truhlar
Refreshments served prior to seminar.