ES2015 Compilation of Abstracts of Invited Speakers and Contributed Talk Speakers

MONDAY, JUNE 22, 2015

Haggett Hall, Cascade Room, University of Washington

	New Methods
Jim Chelikowsky, U of Texas, Austin	“Seeing” the covalent bond: Simulating Atomic Force Microscopy Images
Alexandru Georgescu, Yale U	A Generalized Slave-Particle Formalism for Extended Hubbard Models
Bryan Clark, UIUC	From ab-initio to model systems: tales of unusual conductivity in electronic systems at high temperatures
	Advances in DFT and Applications
Priya Gopal, Central Michigan U	Novel tools for accelerated materials discovery in the AFLOWLIB.ORG repository
Ismaila Dabo, Penn State U	Electronic-Structure Calculations from Koopmans-Compliant Functionals
Eric Bylaska, PNNL	Improving the performance of ab initio molecular dynamics simulations and band structure calculations for actinide and geochemical systems with new algorithms and new machines
	QMC
Hao Shi, College of William & Mary	Recent developments in auxiliary-field quantum Monte Carlo: magnetic orders and spin-orbit coupling
Fengjie Ma, College of William & Mary	Ground and excited state calculations of auxiliary-field Quantum Monte Carlo in solids
Paul Kent, ORNL	New applications of Diffusion Quantum Monte Carlo
	Many Body
Diana Qiu, UC Berkeley	Many-body effects on the electronic and optical properties of quasi-two-dimensional materials
Mei-Yin Chou, Academia Sinica	Dirac Electrons in Silicene on Ag(111): Do they exist?
Emmanuel Gull, U of Michigan	Solutions of the Two Dimensional Hubbard Model

TUESDAY, JUNE 23, 2015

	Dynamics
David Prendergast, LBNL	First-principles explorations of dynamics in materials - from attoseconds to nanoseconds
Shuai Zhang, UC Berkeley	Superionic water at planet interior |an ab initio molecular dynamics study
Jean-Luc Fattebert, LLNL	Truly Scalable O(N) Approach for First-Principles Molecular Dynamics of Non-Metallic Systems
	Ultra-fast and Energy-related
Marco Bernardi, UC Berkeley	Ultrafast Dynamics of Excited Electrons in Semiconductors and Metals for Energy Applications
Kyle Reeves, UNC, Chapel Hill	First-Principles Investigation of Electronic Excitation Dynamics in Water under Proton Irradiation
Alexie Kolpak, MIT	First-principles prediction of oxide surface structure& properties in aqueous electrochemical environments
	Finite Temp and Magnetic Fields
Sam Trickey, U of Florida	Finite-temperature Density Functional Developments and Some Computational Consequences
Bruce Harmon, Iowa State University	LaCoO3 (LCO): electronic structure changes at very high magnetic fields - up to 500T
Michel Côté, Université de Montréal	Electron-phonon coupling and the zero-point phonon renormalization of the electronic band gap
	TDDFT
George Bertsch, U of Washington	Time-dependent Density Functional Theory in the Nonlinear Domain: Successes and Failures
Grigory Kolesov, Harvard U	Time-dependent density functional theory and non-adiabatic Ehrenfest dynamics with localized basis sets
Neepa Maitra, Hunter College	Potentials that Exactly Capture Correlated Electron and Ion Dynamics in Strong Fields
Xiaosong Li, University of Washington	Time-Dependent Two-Component Electronic Structure Theory

WEDNESDAY, JUNE 24, 2015

	Green's Functions
Lucia Reining, Ecole Polytechnique	A direct approach to the calculation of many-body Green's functions
Wenchang Lu, NCSU	Ab initio non-equilibrium Green’s function studies of electronic devices with several thousand atoms
Joshua Kas, U of Washington	Cumulant expansion approaches to excited state electronic structure and spectra
	GW-BSE
Linda Hung, U of Illinois, Chicago	GW-BSE: From Atoms to the Nanoscale
John Vinson, NIST	Using RIXS to probe effects of disorder and quasiparticle lifetime broadening
Feliciano Giustino, U of Oxford	Band structure of plasmonic polarons using the Sternheimer-GW method

Invited Speakers: grey background
Contributed Speakers: white background

*** Abstracts are arranged in order of talk. ***

“Seeing” the covalent bond: Simulating Atomic Force Microscopy Images

James R. Chelikowsky

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Advances in atomic force microscopy (AFM) have made it possible to achieve unprecedented images of covalent bonds, in some cases even to resolve the bond order in polycyclic aromatics. However, fundamental questions remain about interpreting the images and modeling the AFM tip. For example, the bright spots in non-contact AFM images can have a close correspondence to the atomic structure of a given specimen, but there can be contrast changes with tip height that cannot be interpreted directly by atomic positions. While the nature of the tip can be crucial in understanding the details of the image, the atomic structure of the tip is often unknown. This situation is compounded by the difficulty in simulating AFM images. In order to perform computational studies of AFM, one must determine the interatomic forces as a function of the tip height on a fine grid above the specimen.

We propose new high performance algorithms to solve for the quantum forces between the tip and the specimen. This approach coupled with a simple theory that avoids an explicit model of the AFM tip, allows us to replicate accurately AFM images and resolve outstanding issues in their interpretation.

References: T.-L. Chan, C.Z. Wang, K.M. Ho, J.R. Chelikowsky:“Efficient first-principles simulation of noncontact atomic force microscopy for structural analysis,” Phys. Rev. Lett. 102, 176101 (2009) and M. Kim and J.R. Chelikowsky: “Simulated non-contact atomic force microscopy for GaAs surfaces based on real-space pseudopotentials,” Appl. Surf. Sci. 303,163 (2014).

TITLE: 'A Generalized Slave-Particle Formalism for Extended Hubbard Models'

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ABSTRACT:

Correlated electron properties, such as Mott transitions, are long-standing areas of interest in condensed matter physics. Canonical models in this field are (extended) Hubbard models containing localized electronic correlation effects. Slave-boson approaches have long been used for approximate solutions of such models. However, recently, there has been a renaissance of low-cost slave-boson approaches for dealing with correlated transition metal oxide systems.

Two specific models have been used in recent years: the slave-rotor method[1,2,3,4] and the slave-spin approach[5,6]. We introduce a new, general formalism that, in appropriate limits, reproduces these two methods but also permits the creation of a larger variety of other slave-particle approaches and models. The approach corrects a number of errors of the slave-rotor approach due to its inclusion on "unphysical states" while also permitting to employ less complex and detailed descriptions of the slave modes than the slave-spin approach requires. We describe results for Mott transitions in single- and multi-orbital Hubbard models. We also describe how this method can be used to set up and solve many-body models extracted from Wannier analysis of realistic materials such as oxides of nickel.

References:

[1] S. Florens and A. Georges, Phys. Rev. B **66**, 165111 (2002)
[2] S. Florens and A. Georges, Phys. Rev. B **70**, 035114 (2004)
[3] E. Zhao and A. Paramekanti, Phys. Rev. B, **76**, 195101, (2007)
[4] B. Lau and A.J. Millis, Phys. Rev. Lett. **110**, 126404 (2013)
[5] L. de'Medici, A Georges, and S. Biermann, Phys. Rev. B **72**, 205124 (2005)
[6] S. R. Hassan and L. de'Medici, Phys. Rev. B **81** 035106 (2010)

From ab-initio to model systems: tales of unusual conductivity in electronic systems at high temperatures

Bryan Clark, U of Illinois, Urbana Champaign

In this talk, two systems with unusual conductivity at high temperatures will be discussed. First, we highlight our numerical prediction of a new superionic phase in high-temperature, high-pressure ice. This phase is an electronic insulator, but an ionic conductor with highly anisotropic diffusion. Second, we describe a model system with zero conductivity even at infinite temperature, a phenomenon commonly known as many-body localization (MBL). We demonstrate a new method for efficiently and compactly representing the complete spectra of MBL states and show how the phenomenology of MBL follows directly from the properties of these excited states.

Novel tools for accelerated materials discovery in the AFLOWLIB.ORG repository: breakthroughs and challenges in the mapping of the materials genome

Priya Gopal, Central Michigan University

High-Throughput Quantum-Mechanics computation of materials properties by ab initio methods has become the foundation of an effective approach to materials design, discovery and characterization. This data driven approach to materials science currently presents the most promising path to the development of advanced technological materials that could solve or mitigate important social and economic challenges of the 21st century. In particular, the rapid proliferation of computational data on materials properties presents the possibility to complement and extend materials property databases where the experimental data is lacking and difficult to obtain.

Enhanced repositories such as AFLOWLIB, open novel opportunities for structure discovery and optimization, including uncovering of unsuspected compounds, metastable structures and correlations between various properties. The practical realization of these opportunities depends on the the design effcient algorithms for electronic structure simulations of realistic material systems, the systematic compilation and classification of the generated data, and its presentation in easily accessed form to the materials science community, the primary mission of the AFLOW consortium.

Electronic-Structure Calculations from Koopmans-Compliant Functionals

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We derive an orbital-dependent density-functional theory — the *Koopmans-compliant approach*[1,2] — that addresses the main limitations of common functional approximations in describing the complete electronic structure of quantum systems. The Koopmans-compliant method is constructed to enforce piecewise linearity in approximate energy functionals with respect to fractional particle occupations. We illustrate the remarkable performance of this method by comparing predicted molecular photoemission spectra and momentum maps of Dyson orbitals to experimental data, finding excellent agreement with ultraviolet photoemission spectroscopy and orbital tomography measurements,[4,5] while preserving or improving the prediction of total energies and equilibrium geometries.[3] These results highlight the role of Koopmans-compliant functionals as accurate and efficient approximations to the spectral potential.[6]

References

1. I. Dabo, A. Ferretti, N. Marzari, and M. Cococcioni, *Phys. Rev. B* **82,** 115121 (2010).
2. I. Dabo, A. Ferretti, G. Borghi, N. L. Nguyen, N. Poilvert, C. H. Park, M. Cococcioni, and N. Marzari, *Psi-k Newsletter* **119** (2013); I. Dabo, A. Ferretti, and N. Marzari, *Top. Curr. Chem.* **347,** 193 (2014).
3. G. Borghi, A. Ferretti, N. L. Nguyen, I. Dabo, and N. Marzari, *Phys. Rev. B* **90,** 075135 (2014).
4. N. L. Nguyen, G. Borghi, A. Ferretti, I. Dabo, and N. Marzari, *Phys. Rev. Lett.* **114**, 166405 (2015).
5. I. Dabo, A. Ferretti, C.-H. Park, N. Poilvert, Y. Li, M. Cococcioni, and N. Marzari, *Phys. Chem. Chem. Phys.* **15,** 685 (2013).
6. A. Ferretti, I. Dabo, M. Cococcioni, and N. Marzari, *Phys. Rev. B* **89,** 195134 (2014).

TITLE: Improving the performance of ab initio molecular dynamics simulations and band structure calculations for actinide and geochemical systems with new algorithms and new machines

Eric Bylaska, PNNL

Abstract: Methods for directly simulating the behavior of complex strongly interacting atomic systems (molecular dynamics, Monte Carlo) have provided important insight into the behavior of nanoparticles, biochemical systems, actinide systems and geofluids. The limitation of these methods to even wider applications is the difficulty of developing accurate atomic level potential interactions that can capture their complex chemistry. Plane wave DFT methods have provided a means to simulate the both the electronic structure and dynamics from molecules and simple crystals to large nanoscale systems. However, these methods, because of their computational expense, have been limited to smaller systems sizes and short time-scales compared to classical molecular dynamics. Thus the performance of software is always an important consideration and the changing computing technologies based on Intel MICs are requiring major reformulations of our ab initio molecular dynamics and band structure codes.

This talk will focus on our developments in two areas: implementation of plane-wave electronic structure methods into NWChem on hybrid HPC architectures, including exact exchange, fast localization based on the real space density matrix, integration with FEFF, and the development of parallel in time algorithms. The talk will focus on the fundamentals of these methods and the realities in terms of system size, computational requirements and simulation times that are required for their application. Recent applications of these methods will be shown for solvated mineral surfaces and their interaction with metal cations.

Recent developments in auxiliary-field quantum Monte Carlo: magnetic orders and spin-orbit coupling *

Hao Shi and Shiwei Zhang
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We discuss several recent developments in auxiliary field quantum Monte Carlo (AFQMC) for treating magnectic orders and systems with spin-orbit coupling (SOC). Symmetry properties can be preserved via proper choices of the Hubbard-Stratonovich transformation and the trial wave function, to greatly increase the accuracy and efficiency. For example, a generalized Hartree-Fock (GHF) trial wave funtion which perserves symmetry in spin-z direction is shown to further improve the AFQMC accuracy in the Hubbard model compared to standard Hartree-Fock (HF) trial wave functions. We determine the magnetic orders in the ground state of the doped Hubbard model. A formally related development allows AFQMC to treat many-body Hamiltonians with SOC. The random walkers become GHF Slater determinants instead of the usual HF form. With this and several algorithmic advances, we calculate exact properties of the strongly interacting Fermi gas with a Rashba SOC. The interplay between superconductivity and SOC coupling is examined.

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Ground and excited state calculations of auxiliary-field Quantum Monte Carlo in solids[*]

Fengjie Ma, Wirawan Purwanto, Shiwei Zhang, and Henry Krakauer
Department of Physics, College of William and Mary, Williamsburg, VA 23187.

We present recent developments of auxiliary-field Quantum Monte Carlo (AFQMC) calculations for ground and excited state[1] in solids. Two approaches are discussed. In the first, a systematic downfolding method is developed for extended systems, which allows many-body calculations to operate on a simpler and systematically improvable Hamiltonian, while retaining material-specific properties. As a by-product, pseudopotential errors are essentially eliminated using a frozen-core treatment[2]. Dramatic savings of computational cost and excellent accuracy are achieved for a range of solids with AFQMC[3]. With this method, we determine the spin gap in NiO, a challenging material with strong electron correlation effects. In the second approach, we have implemented the recently developed multiple-projector pseudopotentials[4] into planewave based AFQMC (pw-AFQMC), which improves transferability and leads to much smaller planewave cutoff, hence less computational cost, in the pw-AFQMC calculations.

[1] F. Ma, S. Zhang, and H. Krahauer, New J. Phys. 15, 093017 (2013).
[2] W. Purwanto, S. Zhang, and H. Krakauer, J. Chem. Theory Comput. 9, 4825 (2013).
[3] F. Ma, W. Purwanto, S. Zhang, and H. Krakauer, PRL in press (arXiv:1412.0322).
[4] D. R. Hamann, PRB 88, 085117 (2013).

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New applications of Diffusion Quantum Monte Carlo

Paul R. C. Kent

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First principles many-body Quantum Monte Carlo (QMC) methods enable the accurate prediction of electronic structure and offer an increasingly accessible alternative to density functional based methods. However, the applications of QMC have long been restricted to relatively light elements and small systems due to the computational cost. Recently the method is seeing much wider application due to both methodological developments and increased computational power. In this presentation I will discuss the materials and properties that are accessible today, as well as the achievable accuracies. I will give examples from van der Waals systems[1], metal oxides[2,3], and metallic systems relevant for catalysis, and will also outline the opportunities and prospects for reducing the remaining systematic errors in the methodology.

[1] ”Binding and Diffusion of Lithium in Graphite: Quantum Monte Carlo Benchmarks and Validation of van der Waals Density Functional Methods”, P. Ganesh, J. Kim, C. Park, M. Yoon, F. A. Reboredo, and P. R. C. Kent. Journal of Chemical Theory and Computation 10 5318 (2014). http://dx.doi.org/10.1021/ct500617z

[2] “Ab initio quantum Monte Carlo calculations of spin superexchange in cuprates: the benchmarking case of Ca2CuO3”. K. Foyevtsova, J. T. Krogel, J. Kim, P. R. C. Kent, E. Dagotto, and F. A. Reboredo. Physical Review X 4 031003 (2014). http://dx.doi.org/10.1103/PhysRevX.4.031003

[3] “Structural stability and defect energetics of ZnO from diffusion quantum Monte Carlo”, J. A. Santana, J. T. Krogel, J. Kim, P. R. C. Kent, and F. A. Reboredo. Journal of Chemical Physics 142 164705 (2015). http://dx.doi.org/10.1063/1.4919242

Many-body effects on the electronic and optical properties of quasi-two-dimensional materials

Diana Y. Qiu, Felipe H. da Jornada, Ting Cao, Steven G. Louie

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Recently, transition metal dichalcogenides (TMDs), such as MoS_2, $MoSe_2$, WS_2, and WSe_2, have been isolated in mono- and few-layer forms. These atomically-thin materials exhibit many remarkable properties, such as valley-selective optical selections rules and excitons with huge binding energies, and are the subject of intense research interest. We have applied the GW and GW plus Bethe Salpeter equation (GW-BSE) approaches to the electronic and optical properties of these quasi-two-dimensional (2D) materials. We found that the TMDs have multiple series of excitons with binding energies in excess of 0.6 eV, and excitation spectra (excited exciton levels) that cannot be explained by the usual 2D hydrogenic model [1,2]. Both the quasiparticle band gaps and the binding energies are very sensitive to the environment in which the 2D materials are placed. We have also studied excitonic effects and energy loss spectra of electron-hole excitations at finite momentum transfer **q** in the TMDs. We found that the binding energies of the finite center-of-mass momentum excitons (e.g., those corresponding to transitions across the indirect gap with **q**= ½ (Γ➔K) in the Brillouin zone) are as large as those of the direct gap (**q**=0) excitons, and have similarly non-hydrogenic excitation spectra and unusual selection rules. The large binding energies, non-hydrogenic spectra, and the sensitivity of the bandgap and exciton binding energies to substrate screening are all found to be a consequence of a strong spatial variations in the screening of the many-electron interactions due to the quasi-2D nature of the material [3]. These three factors -- i) the necessity to include environmental screening, ii) the strong spatial variations in screening, and iii) the large extent of exciton wavefunctions in real space -- make the study of the optical properties of quasi-2D systems very computationally challenging. For example, it requires in general a sampling of more than 100,000 k-points in the Brillouin zone to obtain converged results. We have developed new interpolation methods and k-point sampling techniques that reduce the computational cost by orders of magnitude, making these studies computationally feasible [4].

This work was supported by NSF grant No. DMR10-1006184 and U.S. DOE under Contract No. DE-AC02-05CH11231.

1. D.Y. Qiu, F.H. da Jornada, and S.G. Louie, "Optical Spectrum of MoS2: Many-body Effects and Diversity of Exciton States," Phys. Rev. Lett. **111**, 216805 (2013).
2. M.M. Ugeda, A.J. Bradley, S-F. Shi, F.H. da Jornada, Y. Zhang, D.Y. Qiu, W. Ruan, S-K. Mo, Z. Hussain, Z-X. Shen, F. Wang, S.G. Louie, and M.F. Crommie, "Giant Bandgap Renormalization and Excitonic Effects in a Monolayer Transition Metal Dichalcogenide Semiconductor," Nature Mat. 13, 1091 (2014).
3. D.Y. Qiu, F.H. da Jornada, and S.G. Louie, in preparation.
4. D.Y. Qiu, F.H. da Jornada, and S.G. Louie, in preparation.

Dirac Electrons in Silicene on Ag(111): Do they exist?

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There have been quite a few experimental attempts to grow silicene on Ag(111) in the past two years. However, there are controversies about whether a silicene layer with mass Dirac fermions actually exists on Ag(111). Chen *et al.* [1] measured the interference patterns in the differential conductance map by scanning tunneling spectroscopy and found a linear dispersion relation as the evidence for massless Dirac fermions. On the other hand, Lin *et al.* [2] found no Landau level sequences appearing in the tunneling spectra under a magnetic field, concluding that the Si-Ag interaction is strong enough to break the symmetry of silicene. In order to resolve these conflicting experimental findings, we have studied various Si/Ag configurations on the surface and their related electronic structures using first-principles density-functional calculations. Comparisons with experimental results will be discussed.

[1] Chen et al. Phys. Rev. Lett. 109, 056804 (2012).
[2] Lin et al., Phys. Rev. Lett. 110, 076801 (2013).

Solutions of the Two Dimensional Hubbard Model: Benchmarks and Results from a Wide Range of Numerical Algorithms

Emmanuel Gull, University of Michigan

Numerical results for ground state and excited state properties (energies, double occupancies, and Matsubara-axis self energies) of the single-orbital Hubbard model on a two-dimensional square lattice are presented, in order to provide an assessment of our ability to compute accurate results in the thermodynamic limit. Many methods are employed, including auxiliary field quantum Monte Carlo, bare and bold-line diagrammatic Monte Carlo, method of dual fermions, density matrix embedding theory, density matrix renormalization group, dynamical cluster approximation, diffusion Monte Carlo within a fixed node approximation, unrestricted coupled cluster theory, and multi-reference projected Hartree-Fock. Comparison of results obtained by different methods allows for the identification of uncertainties and systematic errors. The importance of extrapolation to converged thermodynamic limit values is emphasized. Cases where agreement between different methods is obtained establish benchmark results that may be useful in the validation of new approaches and the improvement of existing methods.

First-principles explorations of dynamics in materials - from attoseconds to nanoseconds - aided by X-ray spectroscopy

David Prendergast
The Molecular Foundry, Lawrence Berkeley National Laboratory

The understanding and control of physical processes relevant to our societal energy needs, encompasses a range of time-scales spanning several orders of magnitude. Here we discuss preliminary work within two limits in this space: light-matter interactions at attosecond timescales and beyond and molecular-scale electrochemical processes at solid-liquid interfaces. Predominantly, we make use of density functional theory approaches, with various extensions designed to model the intrinsic excited states and those of an amazingly versatile probe - X-ray spectroscopy. This talk will focus on our direct interpretations of measurements made using X-ray absorption spectroscopy of the biased gold-water interface [1] and photo-excited silicon [2].

[1] Juan-Jesus Velasco-Velez, Cheng Hao Wu, Tod A. Pascal, Liwen F. Wan, Jinghua Guo, David Prendergast, Miquel Salmeron, The structure of interfacial water on gold electrodes studied by x-ray absorption spectroscopy, Science 346, 831 (2014).
[2] Martin Schultze, Krupa Ramasesha, C.D. Pemmaraju, S. A. Sato, D. Whitmore, A. Gandman, James S. Prell, L. J. Borja, D. Prendergast, K. Yabana, Daniel M. Neumark, Stephen R. Leone, Attosecond band-gap dynamics in silicon, Science 346, 1348 (2014).

TITLE: Superionic water at planet interior conditions—an ab initio molecular dynamics study

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GRANT: Supported by NASA and NSF

ABSTRACT:

The phases and equation of states of water have been of interest in physics and planetary science. Over the past few years, there has been numbers of work on this subject using density functional theory which significantly improve our knowledge in these aspects. This includes new ground-state structures[1], formation of hydrogen-rich non-stoicheometric H-O compounds at 13 Mbar[2], and decomposition into H_2O_2 and a hydrogen-rich phase at 50 Mbar[3], etc. At megabar pressures, with increasing temperature, solid ice transforms into a superionic phase before fully melting. In this superionic phase, the oxygen lattice has been assumed to have bulk-centered cubic symmetry until recently, when a face-centered cubic phase was reported[4]. In this work, we perform molecular dynamics simulations on several different superionic structures and calculate their Gibbs free energy using the thermodynamic integration method. Our result show more possible superionic phases at higher pressures. We also calculated the equation of states for these water phases, which are of importance for modeling the interiors of giant planets such as Uranus and Neptune[5].

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[1] B. Militzer and H. Wilson, PRL **105**, 195701 (2010)

[2] S. Zhang, H. Wilson, K. Driver and B. Militzer, PRB **87**, 024112 (2013)

[3] C. J. Pickard, M. Martinez-Canales, and R. J. Needs, PRL **110**, 245701 (2013)

[4] H. Wilson, M. Wong and B. Militzer, PRL **110**, 151102 (2013)

[5] B. Militzer and S. Zhang, submitted to PRB.

“Truly Scalable O(N) Approach for First-Principles Molecular Dynamics of Non-Metallic Systems”

Jean-Luc Fattebert

We present a scalable O(N) First Principles Molecular Dynamics algorithm based on a non-orthogonal localized orbitals formulation of Density Functional Theory. A scalable strategy is used to approximately compute selected elements of the inverse of the associated overlap matrix. The algorithm, which exploits sparsity and uses nearest neighbor communication only, shows excellent scalability. Accuracy is controlled by the mesh spacing of the finite difference discretization, the size of the localization regions confining the orbitals, and a cutoff radius for the overlap matrix.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Ultrafast Dynamics of Excited Electrons in Semiconductors and Metals for Energy Applications

Dr. Marco Bernardi

How does an excited electron lose its energy? This problem is central in fields ranging from condensed matter physics to electrical engineering and energy. Recently, we developed and applied calculations to study the dynamics of out-of-equilibrium charge carriers – also known as hot carriers – in semiconductors and metals. I will present *ab initio* calculations of electron-phonon, electron-electron, and electron-defect scattering rates that are able to predict the relaxation times and mean free paths of hot carriers in materials.

The talk will discuss application of this framework to three problems: 1) Energy dissipation and hot carrier dynamics in the first picosecond after sunlight absorption in silicon. 2) Hot carrier scattering in GaAs, for which our results contribute to resolve experimental controversies and challenge the common notion that optical lattice vibrations are mainly responsible for hot carrier energy loss. 3) Hot carriers generated by surface plasmon polaritons in noble metals, a process of relevance in optoelectronics, photocatalysis, and photovoltaics, for which our results prescribe optimal conditions for hot carrier generation and extraction, and pave the way to accurate calculations of plasmonic losses in materials.

Taken together, the computational approach presented in this talk shines light on microscopic processes that are hard to capture both with experiments and calculations, and opens new avenues to compute excited electron dynamics in materials.

First-Principles Investigation of Electronic Excitation Dynamics in Water under Proton Irradiation

Reeves, K.G., Kanai, Y.

Keywords: Linear energy transfer (LET), water, particle radiation, RT-TDDFT, non-adiabatic dynamics, electronic transitions

A predictive and quantitative understanding of electronic excitation dynamics in water under proton irradiation is of great importance in many technological areas ranging from proton beam therapy to preventing nuclear reactor damages. Despite its importance, an atomistic description of the excitation mechanism has yet to be fully understood. Identifying how a high-energy ion dissipates its kinetic energy into the electronic subsystem is crucial for predicting atomistic damages, which result in the formation of various radiolytic products.

In this work, we use our new large-scale first-principles Ehrenfest dynamics method [1,2] based on real-time time-dependent density functional theory to simulate the non-adiabatic electronic response of bulk water to a fast proton. In particular, we will discuss the topological nature of the electronic excitation. We will employ maximally-localized Wannier functions to bridge our quantitative findings from our first-principles simulations to the conceptual understanding held in the field of water radiolysis.

[1] "Plane-wave Pseudopotential Implementation of Explicit Integrators for Time-Dependent Kohn-Sham Equations in Large Scale Simulations" A. Schleife, E. W. Draeger, Y. Kanai, A. A. Correa, J. Chem. Phys., 137, 22A546 (2012)

[2] "Quantum Dynamics Simulation of Electrons in Materials on High-Performance Computers" A. Schleife, E. W. Draeger, V. Anisimov, A. A. Correa, Y. Kanai, Computing in Science and Engineering, 16 (5), 54 (2014).

First-principles prediction of oxide surface structure and properties in aqueous electrochemical environments

Alexie Kolpak, Massachusetts Institute of Technology

The design of efficient, stable, and inexpensive catalysts for oxygen evolution and reduction is crucial for the development of electrochemical energy conversion devices such as fuel cells and metal-air batteries. However, such design is often limited by challenges in atomic-scale experimental characterization and computational modeling of solid-liquid interfaces. To address these challenges, we recently proposed a general framework, based on a combination of electronic structure computations and electrochemical principles, for the prediction of oxide surface structure, stoichiometry, stability, and catalytic activity as a function of pH and applied potential. In this talk, we use this approach to demonstrate the critical role of solvated cation species in governing oxide surface composition, and, thereby, surface electronic structure and catalytic activity, in perovskite oxides. We develop environment-structure-property relationships to predict trends in catalyst stability and activity, and show that these relationships can be used to understand experimental observations of surface amorphization and oxygen evolution/reduction activity in perovskite oxide-based catalysts. In addition to providing guidance for catalyst design, our work may lead to new electrochemical approaches for tailoring the properties of complex oxide heterostructures.

Finite-temperature Density Functional Developments and Some Computational Consequences

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To study matter from ambient to extreme conditions of pressure and temperature, the best available simulation approach is ab initio molecular dynamics (AIMD). AIMD uses ion-electron forces from Born-Oppenheimer electronic structure calculations. For computational feasibility, free-energy density functional theory is used to calculate the electronic free energy. Doing that introduces two challenges: (1) the accuracy of the required approximate exchange-correlation (XC) density functionals; (2) the KS computational cost-scaling bottleneck (cube of the number of thermally occupied orbitals). I will summarize progress on both.

First, more than thirty years after the ground-state local spin-density approximation (LSDA) XC functional was extracted from purely first-principles Monte Carlo data, we have produced the corresponding finite-temperature LSDA [1]. Comparison with use of a ground-state functional and finite-T density $n(\mathbf{r},T)$ show the importance of the functional's intrinsic T-dependence. Early results from putting this functional into the FEFF9 code will be sketched, along with recent progress on a related finite-T GGA XC functional. Second, I will show AIMD calculations using orbital free DFT (OF-DFT) and our recently developed, fully non-empirical non-interacting free-energy generalized-gradient approximation functional [2] . OF-DFT in principle provides the same quantum statistical mechanics as KS but with computational cost scaling linear with system volume and T-independent. The OF-DFT AIMD calculations use our recently published Profess@QuantumEspresso code system. We are able to recover near KS-DFT equations of state for simple systems.

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[1] V.V. Karasiev, T. Sjostrom, J. Dufty, and S.B. Trickey, Phys. Rev. Lett. **112**, 076403 (2014).

[2] V.V. Karasiev, D. Chakraborty, O.A. Shukruto and S.B. Trickey, Phys. Rev. B **88**, 161108(R) (2013).

$LaCoO_3$ (LCO): electronic structure changes at very high magnetic fields - up to 500T.

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First reported in 1957, LCO is a non-magnetic small gap material at low temperatures; but exhibits magnetic properties at high temperatures and with doping (particularly with Sr[2]). A recent experiment[3] to 500T indicated a magnetic state with ~1.3 Bohr magnetons per Co atom appears above 100T and persists to ~240T, when the moment again increases, up to ~3.8 Bohr magnetons at 500T, where the experiment ended after about 16 microseconds. Our DFT calculations predict a rhombohedral to cubic structural change and agree with the experimental results to 240T, but larger moments at higher fields can only be obtained with larger relative motion of the atoms.

[1] Research at Ames Lab supported by U.S. DOE BES under Grant No. DE-FG02-99ER45761.

[2] S. Melding, et. al., Phys. Rev. Lett. **109**, 109, 157204 (2012).

[3] V.V. Platonov et. al., *Phys. of the Solid State*, v.**54**. No.2, pp-279-282 (2012).

Electron-phonon coupling and the zero-point phonon renormalization of the electronic band gap

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The coupling of electrons to a bosonic field generally causes a renormalization of the energy levels. Whereas in vacuum, the electromagnetic fluctuations lead to the Lamb shift observed in the hydrogen atom levels, in condensed matter, the phonon field renormalizes the band structure, even at zero temperature. Being as large as several hundreds of meV, this renormalization is critical to the predictive power of ab initio calculations when it comes to absorption spectra, photovoltaic materials, or topological insulators. Following the early work of Fan and others in the 1950s, the problem was addressed by Allen, Heine and Cardona, whose theory provides perturbative expressions in terms of the electron-phonon coupling. Using semi-empirical methods, and later on, density functional theory (DFT), the temperature dependence of the band gap could be obtained for several semiconductors. Among those, diamond has become a case study where the zero-point renormalization is as much as half an election volt. The reliability of DFT for the electron-phonon coupling has however been challenged in recent years. Since the scattering of an electron by a phonon probes the excited states of a system, a theory describing this process should rely on an accurate unrenormalized band structure, unlike the one of DFT. A truly ab initio scheme however would rely on many-body perturbation theory. In this presentation, I will report on how a careful treatment using many-body perturbation theory as implemented by the GW approach result in an enhancement of the electron-electron interaction causing a 40% enhancement in the zero-point renormalization (ZPR) in diamond with respect to the usual DFT treatment.

Time-dependent Density Functional theory in the nonlinear domain: successes and failures

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The time-dependent density-functional theory (TDDFT) has been documented as a "pretty good" computational approach for the linear response to external fields, but its utility in the nonlinear domain has not been studied as thoroughly. My talk will consider several nonlinear phenomena and discuss how well the TDDFT performs. The simplest nonlinear observables are hyperpolarizability and nonlinear susceptibility, and here the TDDFT is found to be quite useful. The second area is the interaction of strong laser pulses on media, including coherent phonon generation and field-dependent diectric functions. Here again the TDDFT offers an attractive compromise between computational tractability and predictive power. For some other processes, attempts to use TDDFT have little or mixed success. Namely, attempts to describe Rabi oscillations in the TDDFT framework have been unsuccessful, while attempts to treat the effects of electron relaxation in X-ray absorption spectra (XAS) are mixed. While a TDDFT approach to Langreth's cumulant treatment has been successfully employed to describe inelastic losses, excitonic effects are beyond the reach of TDDFT.

Time-dependent density functional theory and non-adiabatic Ehrenfest dynamics with localized basis sets : method and applications

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Here we present the method of real-time propagation with time-dependent density functional theory (TDDFT) coupled to ionic motion through the mean-field Ehrenfest dynamics approach. The goal of our method is to treat large systems and complex processes, in particular photo-catalytic reactions and electron transfer events on surfaces and thin films. Due to the complexity of these processes, computational simulations are needed to provide insight into the underlying mechanisms and are therefore crucial for the rational design of new materials. Because of short time steps (below 20 *as*) required for electron propagation such simulations are computationally expensive. Our methodology is based on numerical atomic orbital basis sets which results in good computational efficiency. We have also augmented our framework with a number of additional methods and analysis tools such as spherically- averaged and rotationally-invariant DFT+U methods for efficient and accurate treatment of electron correlation in transition metal oxides; a Hirshfeld partitioning scheme for charge tracking and analysis of local dipole contributions and calculation of absorption spectra from real-time TDDFT. We demonstrate an application of our method to photo-catalytic and electron transfer processes on the (110) surface of rutile titanium dioxide. The latter is one of the most thoroughly studied photocatalytic materials with numerous proposed applications, ranging from water photo-oxidation for hydrogen production to cleanup of environmental pollutants and self-cleaning coatings. We apply our method to study methoxy to formaldehyde photo-catalytic conversion on the surface of titania[1] and electron transfer in a model dye-sensitized solar cell consisting of titania and a perylene chromophore. These simulations unveil the mechanism of the photo-catalytic reaction[2] and demonstrate the critical impact that formation of small polarons has in both examples. In both presented simulations polarons act as strong traps that facilitate the methoxy to formaldehyde conversion reaction and impede perylene-to-titania electron transfer while subsequently allowing for higher electron-hole recombination rates.

[1] Phillips, K. R., Jensen, S. C., Baron, M., Li, S.-C. & Friend, C. M. Sequential photo-oxidation of methanol to methyl formate on TiO2 (110). Journal of the American Chemical Society 135, 574-577 (2013).

[2] Kolesov G., Vinichenko D., Tritsaris G.A., Friend, C. M. & Kaxiras E. Anatomy of the photochemical reaction: excited-state dynamics reveals the C−H acidity mechanism of methoxy photo-oxidation on titania. Journal of Physical Chemistry Letters, 6, 1624−1627 (2015).

Potentials that Exactly Capture Correlated Electron and Ion Dynamics in Strong Fields

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The study of electron dynamics far from the ground-state is of increasing interest today in many applications: attosecond control and manipulation of electron and consequent ion dynamics, photovoltaic design, photoinduced processes in general. Time-dependent density functional theory is a good candidate by which to computationally study such problems. Although it has had much success in the linear response regime for calculations of excitation spectra and response, its reliability in the fully non-perturbative regime is less clear, although increasingly used. By studying some exactly-solvable models of charge-transfer dynamics and strong-field processes, we find that the exact correlation potential of time-dependent density functional theory develops stark features in time that are missed by the currently available approximations. We discuss these features and their implications for charge-transfer dynamics and time-resolved spectroscopy. In the second part of the talk, we broaden our focus to the description of coupled electron-ion motion. When the coupling to quantum nuclear dynamics is accounted for, we find additional terms in the potential acting on the electronic subsystem, that fully account for electron-nuclear correlation, and that can yield significant differences to the traditional potentials used when computing coupled electron-ion dynamics. We study such potentials for the phenomena of field-induced electron localization, and charge-resonance enhanced ionization, within the exact-factorization approach to coupled electron-ion dynamics.

[1] *Time-resolved spectroscopy in time-dependent density functional theory: An exact condition*, J. I. Fuks, K. Luo, E. D. Sandoval, N. T. Maitra, Phys. Rev. Lett. (May 8 issue, 2015) and arXiv:1412.0586

[2] *Dynamics of charge-transfer processes with time-dependent density functional theory*, J. I. Fuks, P. Elliott, A. Rubio, and N. T. Maitra, J. Phys. Chem. Lett. **4**, 735 (2013).

[3] *Exact Factorization of the Time-Dependent Electron-Nuclear Wavefunction*, A. Abedi, N. T. Maitra, and E. K. U. Gross, Phys. Rev. Lett. **105**, 123002 (2010).

[4] *Exact Electronic Potentials in Coupled Electron-Ion Dynamics,* Y. Suzuki, A. Abedi, N. T. Maitra, K. Yamashita, and E.K.U. Gross, Phys. Rev. A. **89**, 040501(R) (2014)

[5] *Charge-Resonance Enhanced Ionization Beyond the Quasistatic Model: Insights from the Exact Factorization Approach*, E. Khosravi, A. Abedi, and N. T. Maitra, submitted (2015).

Time-Dependent Two-Component Electronic Structure Theory

Xiaosong Li, University of Washington

We have formulated an ab initio time-dependent two-component spinor method to study the non-collinear spin dynamics of many-electron systems. We employed a direct integration of the time-dependent non-relativistic two-component Hartree-Fock/Kohn-Sham equation using atom-centered basis functions and a unitary propagation approach with a modified midpoint algorithm. An analysis tool based on the Hirshfeld partitioning scheme has been developed to analyze the time-dependent spin magnetization. For the simple one-electron system of the hydrogen atom and collinear multi-electron system of the lithium atom, the real-time two-component Hartree-Fock simulations yield the same results as the analytical Larmor precessions. As an important application of our methodology, we have simulated spin dynamics of a non-collinear Li3 trimer in response to an external magnetic field.
The switching of the magnetization at each lattice node was observed during the dynamical simulation. This method has been extended to the Ehrenfest dynamics framework that can be used to model spin-flip processes in molecular dissociation dynamics.

A direct approach to the calculation of many-body Green' s functions

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Many-body perturbation theory is a powerful approach to understand and predict many properties of materials. However, sometimes low-order perturbation expressions for the self-energy, like the GW approximation [1] and related approaches, are not sufficient. For example, satellite structure beyond the quasi-particle peaks in the spectral function is often not well described in GW, and in the case of strong coupling, where the quasi-particle picture is no longer adequate, other approaches are needed. We explore an alternative route to the calculation of interacting electron Green's functions. It is based on a set of functional differential equations relating the one-body Greens function to its functional derivative with respect to an external perturbing potential [2]. This set of equations can be used to generate the perturbation series. Here we will show that working directly with the differential equations, instead of some low order approximation to the solution, yields precious insight concerning fundamental questions, guidelines for practical calculations, and methods that lead to an improved description of spectra and total energies. Results will be illustrated on various levels of approximation, ranging from simple models [3] to full ab inito calculations [4].

[1] L. Hedin, Phys. Rev. 139, A796 (1965).
[2] L.P. Kadanoff and G. Baym, Quantum Statistical Mechanics (New York: Benjamin, 1962)
[3] G. Lani, P. Romaniello, and L. Reining, New J. Phys. 14, 013056 (2012); J.A. Berger et al., New J. Phys. 16, 113025 (2014)
[4] M. Guzzo et al., Phys. Rev. Lett. 107, 166401 (2011); Phys. Rev. B 89, 085425 (2014)

Ab initio non-equilibrium Green’s function studies of electronic devices with several thousand atoms

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Multi-probe non-equilibrium Green’s function (NEGF) method has been implemented in our massively parallel DFT-based software, the real space multigrid (RMG) method. Multiple levels of parallelization are used to run efficiently on supercomputers: MPI between nodes, OpenMP in a node, and Cuda for GPU accelerators. Localized atom-centered orbitals, variationally optimized for the lead and conductor regions, respectively, serve as the basis set for NEGF calculations. We describe two applications:

(i) Graphene-based FET transistors

Two-dimensional materials, such as graphene and molybdenum disulfide, have attracted much attention because of their unique properties. Graphene's high mobility make it a very promising material for next generation electronics, but its zero band gap is a hurdle for digital transistors. However, graphene nanoribbons can exhibit band gaps due to quantum confinement, and their electronic properties differ depending on the structures of their edges. Here we systematically study transport properties of graphene-based transistors with up to 5,000 atoms, investigating the effects of nanoribbon index, length, width and gate structure. Surprisingly, we find the that mod(n,3)=0 armchair ribbons would perform best in FET configurations.

(2) Si nanowire p-n junction

With the implemented multi-level parallelization, we are able to simulate two-terminal systems with over 10 thousand atoms. As a first example, we calculated the I-V characteristics of a Si nanowire p-n junction. The nanowire is along the (110) direction in order to minimize the number dangling bonds on the surface. Its diameter is 3 nm. It turns out that due to the long screening length in Si, a channel length of ~24 nm is necessary to observe ideal diode characteristics: exponential current increase in forward bias and nearly zero current with backward bias.

Cumulant expansion approaches to excited state electronic structure and specta

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Cumulant expansions for the one electron Green's function have recently had great success in describing many-body excitations in a variety of materials and spectra.[1,2,3,4] In particular, in comparison to the GW method, improved agreement is found for satellite peaks in x-ray photoemission spectra. However, previous treatments based on expansions of the time-ordered Green's function were inconsistent, failing to describe satellites on both sides of the chemical potential, leading to occupation numbers which retain their free electron values, in contrast to QMC calculations and experimental results. Recent theoretical developments give a consistent picture based on an expansion of the retarded one electron Green's function []. Here we describe several methods for obtaining excited state electronic structure and spectra using cumulant expansion based approaches. First, we describe an extended derivation of the retarded cumulant expansion method which allows for the use of quasiparticle self-consistent starting points.[6] The effects of various levels of self-consistency on quantities of interest, such as spectral functions, quasiparticle properties, and occupation numbers are investigated and discussed. Results are shown for a variety of materials, including semi-conductors and oxides.

Second, we present a real-time TDDFT method for calculating the cumulant for the deep-hole Green's functions. This method has been successful in treating charge-transfer excitations in x-ray emission. Here we extend the treatment to describe x-ray absorption as well, and give results for correlated materials such as transition metal oxides and CeO2.

1. F. Aryasetiawan, L. Hedin, and K. Karlsson, Phys. Rev. Lett. **77**, 2268 (1996)
2. Guzzo et al, Phys. Rev. Lett. **107** 166401 (2011)
3. Johannes Lischner, Derek Vigil-Fowler, and Steven G. Louie, Phys. Rev. Lett. **110**, 146801 (2013)
4. J. J. Kas, F. D. Vila, J. J. Rehr, and S. A. Chambers, Phys. Rev. B **91**, 121112(R) (2015)
5. J. J. Kas, J. J. Rehr, and L. Reining, Phys. Rev. B **90**, 085112 (2014)
6. M. van Schilfgaarde, Takao Kotani, and S. Faleev, Phys. Rev. Lett. **96**, 226402 (2006)

GW-BSE: From Atoms to the Nanoscale

Linda Hung

The GW approximation, coupled with the Bethe-Salpeter equation (BSE), allows the first-principles prediction of electronic and optical properties. In this presentation, we examine the efficiency and accuracy of GW-BSE applied to finite systems such as atoms, molecules, or nanocrystals. After a brief introduction of the GW-BSE theory, we discuss how a real-space basis, with wave functions defined on a spherical uniform grid, takes advantage of quantum confinement to improve computational efficiency. We present simulations predicting the excited-state properties of titanium dioxide nanocrystals up to ~1.5 nm in size. We also benchmark GW and GW-BSE energies on test sets consisting of transition metal atoms, some of their oxide dimers, and organic molecules, with comparison to other software packages and to experiment. Finally, we explore how a LDA-derived vertex function affects the accuracy of quasiparticle and absorption energies on the same benchmark set.

“Using RIXS to probe effects of disorder and quasiparticle lifetime broadening”

John Vinson, NIST

We present measurements and calculations of x-ray absorption (XAS) and resonant inelastic x-ray scattering (RIXS) at the nitrogen K edge of ammonium nitrate. The spectra highlight shortcomings of traditional assumptions used in x-ray spectroscopy calculations. We see unexpectedly large, peak-dependent effects from both vibrational disorder and quasi-particle lifetimes. Notably, the emission from the NO sigma bonds is extremely broad despite almost no dispersion in the band structure. *GW* calculations reveal that this is a characteristic of the quasi-particle state whereby a hole in the sigma bond has a characteristic lifetime less than 1/10th that of the nitrogen 1s hole.

Band structure of plasmonic polarons using the Sternheimer-GW method

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During the past two decades the GW method witnessed significant growth within the electronic structure community. Besides its predictive power in the calculation of quasiparticle band structures, the GW method is appealing since it does not require the use of adjustable parameters. Despite these successes GW calculations suffer from the slow convergence of quasiparticle energies with respect to the number of unoccupied Kohn-Sham states. In order to circumvent this difficulty we developed the so-called 'Sternheimer-GW' method, which avoids the explicit computation of unoccupied Kohn-Sham states [1,2]. In Sternheimer-GW both the screened Coulomb interaction W and the electron Green's function G are evaluated using only occupied Kohn-Sham states, precisely as in density-functional perturbation theory. In this talk I will review the basics of Sternheimer-GW, and discuss comparisons with calculations based on the standard sum-over-states approach. In addition I will discuss one recent application to the calculation of complete energy- and momentum-resolved spectral functions of semiconductors such as three-dimensional bulk silicon and two-dimensional transition metal dichalcogenides. Here, by using Sternheimer-GW in conjunction with the cumulant expansion approach, we have found dispersive photoemission satellites associated with electron-plasmon interactions. The energy vs. momentum dispersion relations of these plasmonic structures closely resemble the standard valence bands, although they are broadened and blue-shifted by the plasmon energy [3].

[1] F. Giustino, M. L. Cohen, S. G. Louie, Phys. Rev. B 81, 115105 (2010).
[2] H. Lambert, F. Giustino, Phys. Rev. B 88, 075117 (2013).
[3] F. Caruso, H. Lambert, F. Giustino, Phys. Rev. Lett. (2015), in press.