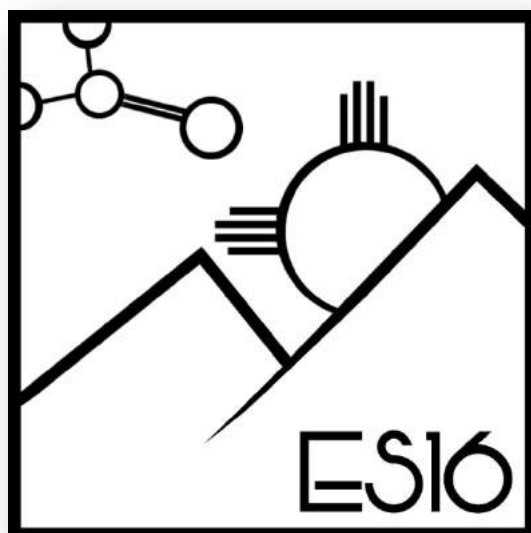


ES2016: The 28th Annual Workshop on Recent Developments in Electronic Structure Methods

June 26-29, 2016
University of New Mexico
Albuquerque, NM 87131, USA



We gratefully acknowledge support of the ES2016 Workshop by the following:



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Los Alamos National Laboratory



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Department of Energy



NSF award from the Materials
Computation Center, University of
Illinois, Urbana-Champaign



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ES2016: The 28th Annual Workshop on Recent Developments in Electronic Structure Methods

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SCHEDULE OF EVENTS

Sunday, June 26

2 PM – 6 PM	Conference check-in and dorm key pickup (Casas del Rio main building [Jemez])
6 PM – 9 PM	Welcome Reception and hosted bar (Casas del Rio Gila/Pecos courtyard)

SCIENTIFIC PROGRAM (SMLC Auditorium)

Note: If you are presenting a poster, please consult the Program Book to find your session number (I or II) and poster number assignment. You may set up your poster starting at 7:30 AM on the day of your session in the SMLC foyer; pins and Velcro will be available at the registration desk.

Monday, June 27

7 AM – 8:30 AM	Conference check-in and breakfast (SMLC foyer)
8:30 AM – 8:45 AM	Welcome; Opening Remarks, Dr. Patricia A. Henning , Interim Associate Vice President for Research (SMLC Auditorium)
8:45 AM – 9:20 AM	Special talk: Mel Levy , <i>On variational principles in time-independent density functional theory</i>
9:20 AM – 9:30 AM	Break
Technical Session I: TDDFT, range-separation, and excited state properties (Chair: Rudy Magyar)	
9:30 AM – 10:05 AM	Carsten Ullrich , <i>Excitons in solids: TDDFT versus many-body perturbation theory</i>
10:05 AM – 10:40 AM	Sivan Refaely-Abramson , <i>Solid-state excitations from density-functional theory</i>
10:40 AM – 11:00 AM	Coffee break (SMLC foyer)
11:00 AM – 11:35 AM	Julien Toulouse , <i>Combining density functional theory and many-body methods</i>

11:35 AM – 12:10 PM	Svetlana Kilina , <i>Theoretical insights into the surface chemistry and its effect on the excited state and its coherent properties in nanomaterials</i>
12:10 PM – 1:40 PM	Lunch (SMLC foyer)
Technical Session II: Algorithms and Methods (Chair: Jerry Bernholc)	
1:40 PM – 2:15 PM	Roland Assaraf , <i>Computing efficiently energy derivatives in quantum Monte Carlo with multi-determinant expansions</i>
2:15 PM – 2:50 PM	Deyu Lu , <i>Local representation of the dielectric response: Theory and applications</i>
2:50 PM – 4:20 PM	Poster Session I and Reception
4:20 PM – 4:55 PM	Volker Blum , <i>All-electron electronic structure pathway to challenges in molecules, materials and “energy”</i>
4:55 PM – 5:30 PM	Christian Negre , <i>Next-generation quantum based Born-Oppenheimer molecular dynamics: Towards hundred-thousand atoms over nanoseconds of time evolution</i>
Evening free	
5:45 PM – 7:30 PM	<p>ES '16 optional tutorial: Real Space Multigrid (RMG) open source electronic structure code, Version 2.0.</p> <p>Jerry Bernholc, Emil Briggs, Wenchang Lu, Miro Hodak</p> <p>RSVP: Emil Briggs, elbriggs .at. ncsu.edu Location: SMLC Room 120. Free pizza will be provided.</p>

Tuesday, June 28

7:00 AM – 8:30 AM	Conference check-in and breakfast (SMLC foyer)
8:30 AM – 9:05 AM	Special talk: Marcus Knudson , <i>Dynamic compression experiments on deuterium and their implications for first-principles theory</i>

9:05 – 9:15 AM	Break
Technical Session III: Bridging Length and Time Scales in Complex Materials (Chair: Blas Uberuaga)	
9:15 – 9:50 AM	Cormac Toher , <i>Progress in automatic quantum mechanical calculations of materials thermodynamics</i>
9:50 AM – 10:25 AM	Max Amsler , <i>Materials Genome and structure optimization: Theory and application of structural optimization via minima hopping</i>
10:25 AM – 10:45 AM	Coffee break (SMLC foyer)
10:45 AM – 11:20 AM	Alan Wright , <i>Density-functional theory investigation of point defects in GaAs</i>
11:20 AM – 11:55 AM	Ching-Ming Wei , <i>Quantum Monte Carlo studies of interactions in van der Waals bilayer systems</i>
11:55 AM – 12:10 PM	Workshop photo
12:10 PM – 1:40 PM	Lunch (SMLC foyer)
Technical Session IV: Electronic Ordering and Strong Correlations (Chair: Warren Pickett)	
1:40 PM – 2:15 PM	Hardy Gross , <i>Ultrafast laser-induced demagnetization of solids: Understanding the mechanism with real-time TDDFT</i>
2:15 PM – 2:50 PM	Julie Staunton , <i>Complex magnetism of lanthanide intermetallics and the role of their valence electrons</i>
2:50 PM – 4:20 PM	Poster Session II and Coffee
4:20 PM – 4:55 PM	Jian-Xin Zhu , <i>Electronic correlation effects in plutonium metals and compounds</i>
4:55 PM – 5:30 PM	Hitesh Changlani , <i>Density-matrix based determination of low-energy model Hamiltonians from ab initio wave functions</i>

6 PM – 10 PM	Reception and hosted bar followed by Workshop banquet (<i>Hodgin Hall</i>)
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Wednesday, June 29

7:00 AM – 8:30 AM	Breakfast (<i>SMLC foyer</i>)
8:30 AM – 8:45 AM	Poster award presentations
Technical Session V: Electronic Structure and Entanglement (Chair: Andrew Baczewski)	
8:45 AM – 9:20 AM	Norm Tubman , <i>Quantum dissection of a covalent bond</i>
9:20 AM – 9:55 AM	Tao Xiang , <i>Renormalization of tensor network models</i>
9:55 AM – 10:25 AM	Coffee break (<i>SMLC foyer</i>)
Technical Session VI: Topological Quantum Materials (Chair: Andrew Rappe)	
10:25 AM – 11:00 AM	Barry Bradlyn , <i>New frontiers for topological semimetals</i>
11:00 AM – 11:35 AM	Youngkuk Kim , <i>Nonsymmorphic Dirac and double Dirac semimetals</i>
11:35 AM – 11:50 AM	Closing remarks and farewell

Invited Talk Abstracts

(in alphabetical order of speaker last name)

Materials Genome and Structure Optimization: Structure Prediction in Materials Design

Maximilian Amsler and Chris Wolverton

*Department of Materials Science and Engineering, Northwestern University
Evanston, IL, USA*

Materials science is one of the most rapidly growing fields in condensed matter physics and chemistry, and has devoted itself to discover functional materials for various technologically-relevant applications. Recently, novel approaches in computational materials science have led to significant advances in materials design, including high-throughput calculations, data-mining and machine learning¹. Another increasingly popular technique is *ab-initio* structure prediction, such as the Minima Hopping Method², which implements a highly efficient global geometry optimization algorithm to identify thermodynamically stable and metastable compounds. I will illustrate how this method can be used to tackle various materials design challenges from different perspectives, supported by examples of its recent, successful application.

- [1] James E. Saal, Scott Kirklin, Muratahan Aykol, Bryce Meredig, and Chris Wolverton, JOM **65**, 15011509 (2013).
- [2] Maximilian Amsler and Stefan Goedecker, J. Chem. Phys. **133**, 224104 (2010).

Computing efficiently energy derivatives in quantum Monte Carlo with multi-determinant expansions.

Roland Assaraf, Claudia Filippi and Saverio Moroni.

*Laboratoire de Chimie Théorique, Université Pierre et Marie Curie, CNRS,
Sorbonne Universités
Paris, France*

We present recent advances for computing with quantum Monte Carlo methods energy derivatives and properties (interatomic forces and so on), with a multi-determinant Jastrow-Slater wave function. The computational scaling as a function of the number N_e+1 of determinants is reduced to $O(N_e)$ per derivative¹, down from $O(NN_e)$ ² where N is the number of electrons. Our formulas use simple matrix algebra, and recover the efficiency of the less transparent algorithmic differentiation technique for one single determinant ($N_e = 0$). We also show that the scaling can be further reduced from $O(N_e)$ per derivative to $O(N_e)$ for the entire set of derivatives³. In practice the extra cost of an expansion ($N_e > 0$) on the numerical scaling is only $O(N_e)$ per Monte Carlo step, independently of the number of derivatives.

- [1] C. Filippi, R. Assaraf and S. Moroni, J. Chem. Phys. **144**, 194105 (2016).
- [2] K. Clark, M. A. Morales, J. McMinis, J. Kim, and G. E. Scuseria, J. Chem. Phys. **135**, 244105 (2011).
- [3] In preparation.

All-electron Electronic Structure Pathway to Challenges in Molecules, Materials and “Energy”

Volker Blum

*Department of Mechanical Engineering and Materials Science, Duke University
Durham, NC, USA*

This talk describes recent advances of all-electron electronic structure methods as implemented in the FHI-aims code, covering semilocal and hybrid DFT for periodic and non-periodic systems on equal footing, as well as many-body perturbation theory such as the random-phase approximation and *GW*. Our approach builds on numerically tabulated atom-centered basis sets,[1] which facilitate very high numerical accuracy,[2] but that can also be employed for routine production simulations up to very large, complex solid or molecular systems (1,000s of atoms). Key methodological components that will be discussed include: The massively parallel eigenvalue solver library ELPA; a new electronic structure infrastructure “ELSI” that will bundle approaches to solve or circumvent the DFT eigenvalue problem towards even larger systems; and an accurate, localized resolution of identity strategy for the two-electron Coulomb operator that facilitates all-electron $O(N)$ hybrid DFT calculations up to 1,000 atoms,[3,4] as well as many-body theory beyond DFT. Finally, we show how these developments enable us to make accurate predictions for complex, nanostructured materials, particularly electronically tunable, crystalline organic-inorganic hybrid materials of interest for photovoltaic or optoelectronic applications.

- [1] V. Blum *et al.*, *Comput. Phys. Commun.* **180**, 2175-2196 (2009).
- K. Lejaeghere *et al.*, *Science* **351** (2016), DOI: 10.1126/science.aad3000
- [3] S. Levchenko *et al.*, *Comput. Phys. Commun.* **192**, 60-69 (2015).
- [4] A. Ihrig *et al.*, *New J. Phys.* **17**, 093020 (2015).

New Frontiers for Topological Semimetals

Barry Bradlyn

Princeton Center for Theoretical Science
Princeton University, Princeton, NJ 08544

Following their insulating counterparts, topological semi-metals have attracted much theoretical and experimental interest. Weyl and Dirac semimetals have recently been theoretically predicted and experimentally observed; both display topologically protected Fermi-arc surface states, as well as large negative magnetoresistance due to the “chiral anomaly.” In this talk, I will discuss two new avenues for finding topological phenomena in gapless materials. First, I will go beyond Weyl and Dirac fermions to discuss how non-symmorphic crystal symmetries can stabilize topological band degeneracies in spin-orbit coupled materials. Some notable consequences of these degeneracies are the presence of Fermi arcs in non-Weyl systems, the fermionic spin-1 generalization of a Weyl fermion, and the existence of Dirac lines. I will pay particular attention to experimentally realizable material candidates. Time permitting, I will also discuss how an external magnetic field can be used to create a Weyl semimetal from a topologically trivial material, and I will show how this lends insight into recent experiments on the half-Heusler GdPtBi.

Density-matrix based determination of low-energy model Hamiltonians from ab initio wavefunctions

Lucas K. Wagner, Huihuo Zheng, Kiel Williams, and Hitesh J. Changlani

*Department of Physics, University of Illinois at Urbana-Champaign
Urbana, Illinois, USA*

We propose a way of obtaining effective low-energy Hubbard-like model Hamiltonians from ab initio Quantum Monte Carlo calculations for molecular and extended systems. The Hamiltonian parameters are fit to best match the ab initio two-body density matrices and energies of the ground and excited states, and thus we refer to the method as “ab initio density matrix based downfolding” [1]. We present representative examples where we estimate effective parameters such as the Hubbard U and the Hund’s coupling J , along with providing systematic tests of the validity of a given model. For molecules, such parameterizations enable calculation of excited states that are usually not accessible within ground state approaches. For solids, the effective Hamiltonian enables large scale calculations using techniques designed for lattice models.

- [1] H. J. Changlani, H. Zheng, L. K. Wagner, *J. Chem. Phys.* 143, 102814 (2015).

Ultrafast laser-induced demagnetization of solids: Understanding the mechanism with real-time TDDFT

E. K.U. Gross

Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany

In the past two decades several experiments have demonstrated the laser-induced demagnetization of ferromagnetic solids in less than 100 femto-seconds. This is orders of magnitude faster than magnetic switching in present-day magnetic-field-based technology. To shed light on the underlying microscopic mechanism, we have performed an ab-initio study of Fe, Co, Ni and Cr in short laser pulses, using real-time non-collinear time-dependent spin density functional theory (TDDFT). We show [1] that the demagnetization proceeds in two distinct steps: First, a fraction of the electrons is excited without much change in the total spin polarization. In a second step, the spin magnetic moment of the remaining localized d-electrons decreases through spin-flip transitions induced by spin-orbit coupling. For pulse lengths of a few femto-seconds, the whole process of demagnetization happens in less than 50 femto-seconds. For antiferromagnetic Heusler compounds, such as Mn_3Ga and Ni_2MnGa , an even faster process is found [2] where magnetic moment is transferred from one sublattice to the other. Employing a combination [3] of TDDFT with Optimal Control Theory, we furthermore demonstrate how the demagnetization process can be controlled with suitably shaped laser pulses. Finally, we assess the influence of the approximation used for the exchange-correlation (xc) functional by comparing non-collinear LSDA results with a novel xc functional [4] that exerts a local exchange-correlation torque.

[1] K. Krieger, J.K. Dewhurst, P. Elliott, S. Sharma and E. K. U. Gross. *Laser-induced demagnetization at ultrashort time scales: Predictions of TDDFT*, Journal of Chemical Theory and Computation **11**, 4870 (2015).

[2] P. Elliott, T. Mueller, J. K. Dewhurst, S. Sharma, and E. K.U. Gross. arXiv 1603.05603 (2016).

[3] A. Castro, J. Werschnik, and E. K.U. Gross. *Controlling the dynamics of many-electron systems from first principles: A combination of Optimal Control and Time-Dependent Density-Functional Theory*, Phys. Rev. Lett. **109**, 153603 (2012).

[4] F. G. Eich and E. K. U. Gross. *Transverse spin-gradient functional for noncollinear spin-density-functional theory*, Phys. Rev. Lett. **111**, 156401 (2013).

Nonsymmorphic Dirac and double Dirac semimetals

Benjamin J. Wieder¹, Charles L. Kane¹, Andrew M. Rappe², and
Youngkuk Kim²

¹*Department of Physics and Astronomy, University of Pennsylvania
Philadelphia, Pennsylvania 19104-6323, USA*

²*The Makineni Theoretical Laboratories, Department of Chemistry,
University of Pennsylvania
Philadelphia, Pennsylvania 19104-6323, USA*

Three-dimensional (3D) Dirac semimetals feature a fourfold-degenerate Dirac point at high-symmetric points of the Brillouin zone, protected by nonsymmorphic symmetries of crystals ¹. Here we briefly review the 3D Dirac semimetals and introduce a novel class of Dirac semimetals that feature an eightfold-degenerate double Dirac point ². We show that 7 of the 230 space groups can host such Dirac points and, in particular, space group 135 can host an intrinsic double Dirac semimetal with no additional states at the Fermi energy. This defines a symmetry-protected topological critical point, and a uniaxial compressive strain applied in different directions leads to topologically distinct insulating phases. In addition, the double Dirac semimetal can accommodate topological line defects that bind helical modes. Potential materials realizations are discussed.

- [1] S. M. Young, S. Zaheer, J. C. Y. Teo, C. L. Kane, E. J. Mele, and A. M. Rappe, Phys. Rev. Lett. **108**, 140405-1 (2012).
- [2] Benjamin J. Wieder, Youngkuk Kim, A.M. Rappe, and C.L. Kane, Phys. Rev. Lett. **116**, 186402-1 (2016).

Theoretical insights into the surface chemistry and its effect on the excited state and its coherent properties in nanomaterials

Svetlana Kilina

Chemistry and Biochemistry Department, North Dakota State University,
Fargo, ND 58102, US

We have developed time-domain non-adiabatic dynamics based on density functional theory to determine conditions that govern the mechanisms of exciton relaxation in photoexcited semiconductor quantum dots (QDs) passivated by various ligands. Our approach treats phonons semi-classically, which allows us to explicitly incorporate quantum decoherence effects within the electronic subsystem. Both elastic and inelastic electron-phonon interactions play key roles in solar energy harvesting. Coherence of these processes is very important, because quantum transitions can occur only through buildup of coherence. Our simulations provide fundamental insights into the origin of the pure-dephasing process in the bare and passivated QDs. Thus, we have revealed the role of surface defects and decoherence in the ultrafast loss of photoexcitation to heat in QDs and established a connection between the slow energy relaxation — the phonon bottleneck — and Zeno effect. We also have found that elastic and inelastic scattering respond in the opposite manner to CdSe QD surface passivated by ligands. Phonon-induced pure-dephasing processes determined by elastic electron-phonon scattering in QD capped with ligands are much longer than that in bare QD. The difference is rationalized by the fact that ligands have no direct contributions to the electronic densities of the lower-energy states involved in the superpositions, while they indirectly reduce mobility and fluctuations of the surface atoms. In contrast, the higher-energy electronic states involved in the relaxation are delocalized over ligands and the QD, and therefore, ligands increase the electron-phonon coupling in the case of inelastic processes. We also investigate the effect of the QD-QD interaction on their optical properties. Our calculations suggest that a fast energy transfer between an excited QD to the nearest one provides an additional channel for occupation of long-leaving semi-dark and dark trap states in neighboring QDs forcing the emission to happen from higher-energy optically bright states. This pathway increases 'on' blinking time in aggregates of strongly interacting Si QDs, as experimentally observed. Overall, our calculations provide insights into the surface chemistry of QDs and offering guidance for controlling the optical response of nanostructures by means of OD-QD and QD-ligand engineering.

Dynamic compression experiments on deuterium and their implications for first-principles theory

M.P. Desjarlais,¹ A. Becker,² R.W. Lemke,¹ K.R. Cochrane,¹ M.E. Savage,¹ D.E. Bliss,¹ T.R. Mattsson,¹ R. Redmer,² and Marcus D. Knudson^{1,3}

¹Sandia National Laboratories, Albuquerque, NM, USA

²Institute of Physics, University of Rostock, Rostock, Germany

³Institute for Shock Physics, Washington State University, Pullman, WA, USA

Recently a so-called shock-ramp platform has been developed on the Sandia Z Accelerator to access off-Hugoniot states in liquids. The accelerator delivers a two-step current pulse; the first accelerates the electrode to a reasonably constant velocity, which upon impact with the sample cell creates a well-defined shock, the subsequent current rise produces ramp compression from the initially shocked state. This technique generates relatively cool (~1-2 kK), high pressure (>300 GPa), high compression states (~10-15 fold compression), allowing experimental access to the region of phase space where hydrogen is predicted to undergo a first-order phase transition from an insulating molecular-like liquid to a conducting atomic-like liquid. In this talk we will discuss the experimental platform, survey the various theoretical predictions for the liquid-liquid, insulator-to-metal transition in hydrogen, and present the results of experiments that clearly show an abrupt transition to a metallic state. We will also present recent Hugoniot and reshock data for deuterium with unprecedented precision in the vicinity of the molecular-to-atomic transition. These data not only establish maximum compression along the Hugoniot at 4.5-fold, but also enable high-fidelity comparisons with first-principles theory. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Perspectives on Variational Principles in Time-Independent Density-Functional Theory and Total Energy as a Simple Sum of Shifted Kohn-Sham Orbital Energies

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The early history of density-functional theory shall be explored through personal anecdotes, with emphasis on remembering Walter Kohn. Then the corresponding variational principles for ground states in density and density-matrix functional theories will be reviewed briefly for the non-degenerate and degenerate situations through the general constrained-search formulation [1]. Based on these variational principles, properties of exact functionals will be presented. The implementation of these properties helps in the construction of accurate functionals. Special emphasis will be given to coordinate scaling, potentials (functional derivatives), and fractional electron number.

It has recently been observed [2] that the exact interacting ground-state energy may be obtained, in principle, as a simple sum of orbital energies when a universal density-dependent constant is added to the Kohn-Sham potential or to one of its generalizations. The resultant shifted potential has intriguing features, including the fact that a significant component of it changes relatively little on average when the density changes and the fact that the potential does not undergo a discontinuity when the number of electrons increases through an integer. Thus, the approximation of this shifted potential represents an alternative direct approach for the approximation of the ground-state energy and density.

A time-independent excited-state Kohn-Sham theory will be presented that utilizes special properties of Coulomb systems [3].

[1] For a brief personal account of the extension of the original H-K theorem, to include degeneracies and more through the constrained-search approach, see M. Levy, *Int. J. Quantum Chem.* **110**, 3140 (2010).

[2] M. Levy and F. Zahariev, *Phys. Rev. Lett.* **113**, 113002 (2014).

[3] P. W. Ayers, M. Levy, and A. Nagy, *J. Chem. Phys.* **143**, 191101 (2015); *Phys. Rev. A.* **85**, 042518 (2012).

Local representation of the electronic dielectric response function: Theory and applications

Deyu Lu

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The microscopic electronic dielectric response function is a central physical quantity that captures the many-electron correlation effects in the ground state total energy and electronic excitations. Key quantities include molecular polarizabilities in different chemical environments, the correlation energy under the random phase approximation, and the screened Coulomb interaction under the GW/BSE framework. Although it is non-local by definition, a local representation of the dielectric response function in real space can provide insightful understanding of its chemical nature and improve the computational efficiency of first principles excited state methods. Recently we proposed a local representation of the electronic dielectric response function [1], based on a spatial partition of the dielectric response into contributions from each occupied Wannier function using a generalized density functional perturbation theory. We show that the locality of the bare response function is determined by the locality of three quantities: Wannier functions of the occupied manifold, the density matrix, and the Hamiltonian matrix. In systems with a gap, the bare dielectric response is exponentially localized, which supports the physical picture of the dielectric response function as a collection of interacting local response that can be captured by a tight-binding model. Several applications of the local response theory will be discussed including response density partition, bond polarizability, dielectric band structure interpolation, and molecular polarizability in condensed phase.

This research used resources of the Center for Functional Nanomaterials, which is a U.S. DOE Office of Science Facility, at Brookhaven National Laboratory under Contract No. DE-SC0012704.

[1] X. Ge and D. Lu, Phys. Rev. B 92, 241107(R), 2015.

Next generation quantum based Born-Oppenheimer molecular dynamics: Towards hundred thousand atoms over nanoseconds of time evolution.

Christian F. A. Negre, Susan. M. Mniszewski, Nicolas Bock, Michael Wall,
Marc J. Cawkwell, Anders M. N. Niklasson

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We have developed a modern framework for Quantum Molecular Dynamics (QMD) simulation based on an Extended Lagrangian formulation of Born-Oppenheimer MD. This allows for the first time energy conserving MD simulations with a linear scaling computational cost. Moreover, the iterative self-consistent field (SCF) optimization required prior to the force evaluations can be avoided and typically only a single Hamiltonian (H) construction and diagonalization is necessary at each time step.

For the linear scaling electronic structure solver, we use either a recursive Fermi operator expansion (SP2) that exploits the underlying matrix sparsity, or a graph-based approach where the calculations are distributed across multiple nodes following a predicted data dependency graph.

The SP2 algorithm allows us to compute the density matrix ρ directly without the need of diagonalizing H . The underlying sparsity of the Fermi operator expansion combined with efficient thresholded sparse matrix-matrix multiplication algorithms gives rise to a linear dependence of the cost with a well-controlled and tunable accuracy.

The graph-based approach provides a highly scalable natural parallelism combined with a tunable well-controlled accuracy of a thresholded sparse matrix algebra. In a single point calculation of a 20,000 atoms complex biosystem we achieve sub-second wall-clock time in the calculation of the density matrix on a 32-node architecture.

By reducing the number of SCF cycles yet maintaining a long-term energy stability with the Extended Lagrangian formulation; and distributing the calculation across multiple nodes with the linear scaling graph-based approach, practical QMD simulations of million atom biomolecular systems are within reach in the very near future.

Solid-State Excitations from Density-Functional Theory

Sivan Refaely-Abramson,^{1*} Manish Jain,² Sahar Sharifzadeh,³ Jeffrey B. Neaton,⁴
and Leeor Kronik¹

¹ Dept. of Materials and Interfaces, WIS, Rehovoth, Israel

² Dept. of Physics, IISc, Bangalore, India

³ Dept. of Electrical and Computer Engineering and Physics Division of Materials Science and
Engineering, BU, Boston, USA

⁴ Dept. of Physics, UCB, Molecular Foundry, LBNL, and Kavli Energy NSIB, Berkeley, USA

The development of a non-empirical theory for quantitative electronic structure calculations, which combines predictive power with computational simplicity, is a long-standing challenge for computational studies in materials science, solid-state physics, and chemistry. In this talk I will present a new framework for obtaining reliable solid-state charge and optical excitations and spectra from an optimally tuned screened range-separated hybrid density functional, which allows for an accurate prediction of exciton binding energies. I will demonstrate this approach through first principles calculations of one- and two-particle excitations in organic semiconductors, fully from first-principles. I will further show that with one adjustable parameter, this method accurately predicts band structures and optical spectra of silicon and lithium fluoride, prototypical covalent and ionic solids. These findings indicate that for a broad range of extended bulk systems, this method may provide a computationally inexpensive alternative to many-body perturbation theory, opening the door to studies of materials of increasing size and complexity [1].

[1] S. Refaely-Abramson, M. Jain, S. Sharifzadeh, J. B. Neaton, and L. Kronik, *Solid-state optical absorption from optimally tuned time-dependent range-separated hybrid density functional theory*, Phys. Rev. B **92**, 081204(R) (2015).

* Present address: Dept. of Physics, UCB, and Molecular Foundry, LBNL, Berkeley, CA, USA

The complex magnetism of lanthanide intermetallics: ab-initio disordered local moment theory

L. Petit, D. Paudyal, Y. Mudryk, K. A. Gschneidner Jr., V. K. Pecharsky,
M. Lüders, Z. Szotek, R. Banerjee and J. B. Staunton

*Department of Physics, University of Warwick
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The Density Functional Theory (DFT)-based 'disordered local moment' (DLM) picture for magnetism at finite temperatures shows how relatively slowly fluctuating local moments can emerge from the interacting electrons of many materials [1,2]. With a suitable description of the f-electron states, this is a good model for rare earth magnets providing a quantitative description of magnetic ordering and magnetic phase diagrams as demonstrated in an application to gadolinium and the other heavy rare earth elements [3]. We show an ab-initio theory of magnetocaloric effect (MCE) and results for gadolinium [4]. We explore an apparently simple prototypical class of lanthanide magnets (GdZn, GdCd and GdMg) with rich, complex and diverse magnetism. We explain why GdZn and GdCd are simple ferromagnets and predict a remarkably large increase of Curie temperature with pressure for GdCd which has been confirmed experimentally [5]. Moreover we find the origin of a ferromagnetic-antiferromagnetic competition in GdMg manifested by non-collinear, canted magnetic order at low temperatures. Replacing 35% of the Mg atoms with Zn removes this transition in excellent agreement with longstanding experimental data [5].

- [1] B.L. Gyorffy et al., J. Phys. F Met. Phys. **15**,1337, (1985).
- [2] J.B. Staunton et al., Phys Rev B **89**,054427, (2014).
- [3] I.D. Hughes et al., Nature, **446**, 650, (2007).
- [4] J.B. Staunton et al., J. Phys. Condens. Matter **26**,274210, (2014).
- [5] L. Petit et al., Phys. Rev. Lett. **115**, 207201, (2015).

Progress in automatic quantum mechanical calculations of materials thermodynamics

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Many thermodynamic properties of materials can be automatically predicted from DFT calculations through the integrated framework AFLOW [1, 2]. We have implemented automated frameworks to calculate vibrational properties using Debye-Grüneisen models [3], or using finite displacement calculations to obtain the anharmonic interatomic force constants and the phonon modes. We have recently formulated descriptors for configurational and structural entropy based on DFT calculations for different structures and configurations [4]. These results can then be used to predict the properties, stability and synthesizability of materials at finite temperature.

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Combining density-functional theory and many-body methods

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Nowadays, a major strategy for improving approximations in density-functional theory (DFT) is to combine DFT with many-body methods such as many-body perturbation theory. Range separation of the electron-electron interaction provides a practical way of performing such a combination by using a (semi)local-density approximation for the short-range part and an explicit many-body approximation for the long-range part. It combines the best of both worlds: an accurate and compact description of short-range interactions by DFT approximations and an accurate description of long-range nonlocal interactions by many-body approximations, while avoiding any double counting of electron correlations.

After giving an overview of such approaches, I will present some recent advances concerning:

- Range-separated hybrid methods for describing ground-state correlations in molecular and solid-state systems, based on second-order perturbation theory and random-phase approximations^{1,2};
- Range-separated hybrid methods for calculating excitation energies in molecular systems, based a long-range frequency-dependent second-order Bethe-Salpeter correlation kernel³.

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Quantum Dissection of a Covalent Bond

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Theoretical analysis of covalent bonding is quite successful in many regards, but leaves open many mysteries even for simple diatomic molecules. We develop a framework for analyzing bonds which uses ideas from the field of quantum entanglement. The main development involves the creation of tools that break up a many body wave function into real space pieces. This includes a recent algorithm that we developed that is able to calculate the entanglement spectrum with quantum Monte Carlo. We are able to address the controversial C_2 molecule with these tools, and demonstrate its bonding properties, which includes an inverted fourth bond. With this analysis we also consider bonding in Hartree-Fock wave functions and find simple additions to text book molecular orbital theory that can easily be incorporated into molecular hybridization diagrams. The ideas considered in this work have the potential to provide a significantly more detailed picture of bonding than allowed by previous techniques.

Excitons in solids with time-dependent density-functional theory: the bootstrap kernel and beyond

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Time-dependent density-functional theory (TDDFT) is an efficient method to describe the optical properties of solids.¹ Lately, a series of bootstrap-type exchange-correlation (xc) kernels² have been reported to produce accurate excitons in solids, but different bootstrap-type kernels exist in the literature, with mixed results.³ In this presentation, we review and clarify the status of the bootstrap kernels and present a new empirical TDDFT xc kernel to compute excitonic properties of semiconductors and insulators efficiently and accurately. We also discuss the recently proposed nonempirical screened exact-exchange (SXX) approach for excitonic properties,⁴ which can be viewed as a first step towards an excitonic hybrid TDDFT functional. SXX performs well for bound excitons and continuum spectra in both small-gap semiconductors and large-gap insulators, with a computational cost much lower than that of solving the Bethe-Salpeter equation.

This work was supported by NSF Grant DMR-1408904.

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The Quantum Monte Carlo studies of interactions in van der Waals bilayer systems

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The van der Waals (vdW) interaction is one of the most fundamental physical quantities resulting from quantum fluctuation of charges. However, it remains a challenge to account for this interaction quantitatively in both theory and experiment. In recent years, there have been many proposed vdW functionals attempted to overcome this deficiency; however, discrepancies in the obtained binding energies using different vdW functionals are usually apparent.

In this work, we present the results of the binding energy for various two-dimensional (2D) bilayer systems: BN/BN [1], Silicene/BN, Silicene/Graphene, and MoS₂/Graphene using Diffusion Monte Carlo (DMC) and density functional theory (DFT) with LDA, GGA, and various vdW functionals. The DMC results of binding energy and the behavior beyond the equilibrium distance have diverse differences from those obtained by DFT with LDA, GGA, and vdW functionals. The outcome of present study would serve as the benchmark of 2D bilayer systems for various DFT vdW functionals and guidance for prospective experiments.

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Migration Processes of the As Interstitial in GaAs and InGaAs

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Thermal and carrier-induced migration processes of the As interstitial in GaAs have been studied using density-functional theory (DFT) and the local-density approximation (LDA) for exchange and correlation. The most important thermal processes were found to involve the -1, 0 and +1 charge states and to produce migration along $\langle 110 \rangle$ -type directions. In the -1 and 0 charge states, migration proceeds via hops between stable *split-interstitial* configurations at bulk As sites through saddle-point configurations in which the As interstitial *bridges* two adjacent bulk As sites. In the +1 charge state, the roles of these two configurations are approximately reversed and migration proceeds via hops between stable bridging configurations through metastable split-interstitial configurations, which are bounded by slightly distorted split-interstitial configurations. Calculated activation energies for thermal migration in the 0 and +1 charge states are in good agreement with measured activation energies in semi-insulating and *p*-type GaAs. Also consistent with observations, the approximate reversal of the stable-state and saddle-point configurations in the 0 and +1 charge states is found to enable carrier-induced migration via a Bourgoin-Corbett mechanism with a residual activation energy of 0.05 eV.

As interstitial migration via these same thermal and carrier-induced processes has also been studied in an $\text{In}_{0.5}\text{Ga}_{0.5}\text{As}$ alloy. In this case, kinetic Monte Carlo (kMC) simulations are required because the stable-state and saddle-point energies of the As interstitial depend on its nearby group-III site occupations and, hence, on its location in the alloy. To enable these simulations, we developed parameterized models (*cluster expansions*) of the As interstitial stable-state and saddle-point energies in the alloy based on DFT results for *training sets* of alloy configurations having different nearby group-III site occupations. Results from the kMC simulations display qualitatively and consequentially different migration from what is found in GaAs.

This work was supported, in part, by Sandia's Solid-State Lighting Science Energy Frontier Research Center, sponsored by the U.S. Department of Energy, Office of Basic Energy Sciences. This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000.

Renormalization of tensor network states

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Progress in the development and application of the tensor renormalization group for two or three dimensional statistical and quantum lattice models is reviewed. Emphasis is given to the coarse graining tensor renormalization group method using the higher-order singular value decomposition (HOTRG) and the projected entangled simplex representation for the ground state wave function of quantum lattice models. The HOTRG provides an accurate but low computational cost technique for studying both classical and quantum lattice models in two or three dimensions. The projected entangled simplex state (PESS), on the other hand, provides a good representation of tensor network states for highly frustrated quantum lattice models. The PESS extends the pair correlation in the projected entangled pair states (PEPS) to a simplex.

Electronic Correlation Effects in Plutonium Metals and Compounds

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An understanding of the phase diagram of elemental plutonium (Pu) must include both the effects of the strong directional bonding and the high density of states of the Pu $5f$ electrons, as well as how that bonding weakens under the influence of strong electronic correlations. In this talk, I will give an LDA+DMFT perspective on the electronic correlation effects in Pu elemental solids and compounds. After a brief overview of the earlier results of electronic structure calculations on the δ -phase of Pu, I will discuss the Kondo physics of Pu impurity in a non-interacting bath [1], and then proceed to discuss the electronic structure of the true α -phase of Pu [2] and Pu-115 compounds [3]. A further development of the DMFT-based first-principles approach will be briefly discussed.

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Poster Abstracts I
Monday Session

(number indicates poster location)

Correct implementation of polarization constants in wurtzite materials and impact on III-nitrides

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Accurate values for polarization discontinuities between pyroelectric materials are critical for understanding and designing the electronic properties of heterostructures. For wurtzite materials, the zincblende structure has been used in the literature as a reference to determine the effective spontaneous polarization constants. We show that, because the zincblende structure has a nonzero formal polarization, this method results in a spurious contribution to the spontaneous polarization differences between materials. In addition, we address the correct choice of “improper” versus “proper” piezoelectric constants. For the technologically important III-nitride materials GaN, AlN, and InN, we determine polarization discontinuities using a consistent reference based on the layered hexagonal structure and the correct choice of piezoelectric constants, and discuss the results in light of available experimental data.

The Role of Double TiO_2 layers in the monolayer $\text{FeSe}/\text{SrTiO}_3$ superconductor

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The interfacial superconductor consisting of a monolayer of FeSe on SrTiO₃ (STO) has been a focus of much experimental and theoretical interest. In part, this is because the critical temperature can go as high as above liquid nitrogen temperature and is $\sim 10\times$ higher than the bulk FeSe critical temperature (at ambient pressure). The interfacial nature of the superconductivity is thus critical and the subject of intense research. To date, theoretical studies based on density functional theory have had difficulties explaining a key feature in the observed Fermi surface topology of the system, namely the absence of a “hole pocket” about the Γ point in the Brillouin zone of the FeSe and STO subsystem. In a collaborative work with experimental colleagues¹, we have found that the STO surface termination in this system is not the usual 1 single-layer TiO_2 that has been assumed in almost all works to date. Instead, the STO surface has a more complex double-layered TiO_2 structure. Both experiment and theory show that the double layer facilitates the epitaxial growth of the monolayer FeSe. In addition, our calculations reveal that the Γ hole pocket can be eliminated due to the enhanced tendency of the double layer (compared to the single layer TiO_2 termination) to donate electrons to the FeSe when oxygen vacancies are present in the surface TiO_2 layer. We also show that it is always easier to form an oxygen vacancy in a double TiO_2 terminated STO compared to a single TiO_2 terminated STO irrespective of the choice of surface unit cell (1×1 , 2×2 , $c(2\times 2)$ etc.) or the areal density of oxygen vacancies on the surface.

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Spin texture of topological surface states of side-surfaces in Bi_2Se_3 from first principles

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Topological insulators have recently drawn a lot of attention because of topologically protected surface states with Dirac dispersion and spin-momentum locking induced by time-reversal symmetry and strong spin-orbit coupling, respectively. Recent experiments report interesting transport properties of Bi_2Se_3 nanowires and nanoribbons with growth directions normal to the (111) surface. However, most of the studies of Bi_2Se_3 are focused on the (111) surface. Additionally, surfaces other than the (111) surface would facilitate hole doping with adatoms since both Bi and Se atoms are present at these other surfaces. We investigate the spin texture and electronic structure of topologically protected surface states of two representative side-surfaces of Bi_2Se_3 by using density-functional theory (DFT). In particular, we consider two surfaces normal to the (111) surface, such as $(\bar{1}\bar{1}0)$ and $(11\bar{2})$, where the former has twofold symmetry and the latter has mirror symmetry. We present our calculated spin textures of the surface states of these side surfaces that qualitatively differ from typical Rashba-like features and from the prediction based on the bulk model Hamiltonian by keeping up to quadratic terms in momentum.

The stability of anatase $\text{TiO}_{2-x}\text{S}_x$ from the first principles calculations

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Titanium dioxide (TiO_2) is known for its numerous and diverse applications, which range from common products to advanced devices.^[1,2] Usually doping is often used to tune the properties of materials. In this work, S doping in anatase TiO_2 ($\text{TiO}_{2-x}\text{S}_x$) was studied using the first principles calculations method.^[3-5] The total energy calculations were used to determine the defect formation energies and the chemical potential landscape^[6] with different S doping concentrations. Results showed that anatase $\text{TiO}_{2-x}\text{S}_x$ with concentrations $x=0.0278$ and 0.0625 cannot exist without the co-existence of other Ti binary compounds, such as TiO_2 , Ti_2O_3 , TiS , TiS_2 , and TiS_3 . These results offer the reliable explanation and prediction for the related experiments.

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High throughput search of field-induced topological ferroelectrics in ABX_3 (X=Cl,Br,I)

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Using first principles density functional theory calculations, we perform a high throughput search of topological phases in a newly-identified class of ferroelectric and antiferroelectric materials in the Inorganic Crystal Structure Database (ICSD) within the halide ABX_3 (X=Cl,Br,I) family of compounds. Accurate band gaps of selected compounds are obtained with hybrid functionals, including spin-orbit interactions. We find several ABX_3 (X=Cl,Br,I) materials that, upon stabilization in the perovskite structure, display a small energy difference (~ 10 meV) between the polar ferroic $R3c$ ($a^-a^-a^-$ in Glazer notation) and the nonpolar antiferrodistortive $Pnma$ ($a^-a^-b^+$ in Glazer notation) distortions, characteristic of antiferroelectricity. We predict trivial ferroelectrics and antiferroelectrics, whose competing $R3c$ polar phase display promising semiconducting properties for photovoltaic applications such as small band gaps of ~ 1 eV and macroscopic polarization of $\sim 10 \mu C/cm^2$. In addition, we predict that the hypothetical perovskites $RbSnI_3$ and $RbSnBr_3$ are bulk topological insulators in the reference cubic $Pm\bar{3}m$ phase and the metastable polar $R3c$ distortion, but correspond to trivial insulators in the nonpolar $Pnma$ structure. These compounds, are therefore antiferroelectrics that display an induced topological ferroelectric phase, even in the presence of oxygen octahedral rotations, through the application of an external electric field. We explore the structural and electronic properties that lead to such behavior by computing surface states and topological invariants, and suggest possible technological applications, such as switchable photovoltaic devices with combined structural, electronic and optical functionalities.

Charge-transfer embedded atom potentials (CT-EAM): from atoms and ions to amino acids and proteins

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A novel reactive charge transfer force field^[1] for studying the dynamics of atomistic systems, including solvated amino acids and proteins, has been developed based on the embedded-atom method (EAM) pioneered by Daw and Baskes. CT-EAM is an alternative to traditional approaches such as EAM for metals, or CHARMM for biomolecular systems, which do not generalize well and cannot describe chemical bond formation and breaking. CT-EAM addresses these issues by modeling charge distortion and charge transfer in interacting atoms and ions using *pseudoatom* building blocks instead of isolated atoms. Here we report initial results toward the CT-EAM parameterization of the twenty naturally-occurring amino acids. We have constructed a database of known and novel amino acid conformers using an adaptation of the stochastic Saunders method^[2]. Conformer energies, select transition states, and solvation states were identified using Gaussian '09 at the MP2 level of theory, for a set of six exemplar amino acids: glycine, alanine, cysteine, serine, proline and lysine. These energies and corresponding conformer dipole moments will be used to parameterize the CT-EAM potential against isolated amino acid properties (training set), followed by testing against computed 1D cuts through *interacting* amino acid potential energy surfaces. We used 6-311++G(d,p) basis sets that include polarization and diffuse functions for all atoms present. This is particularly important because of the presence of ionic and excited state pseudoatom components in the CT-EAM potential.

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RMG version 2.0 electronic structure code

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RMG (Real-space MultiGrid) is an open source, DFT-based electronic structure code that discretizes the Kohn Sham equations on real-space grids. Either norm-conserving or ultrasoft pseudopotentials are used to represent the atomic species. An extensive default set of pseudopotentials is provided with the download package. The Kohn-Sham equations are solved using *multigrid* preconditioning techniques coupled with subspace matrix diagonalization methods. RMG has been efficiently parallelized for a wide range of computer and cluster architectures. It runs well on systems ranging from standard workstations up to the largest supercomputers available today, where a peak performance in excess of 6.5 Pflops was demonstrated using an earlier version of the code. When present, GPU accelerators can be used to improve performance. Both Nvidia and Intel variants are supported.

Version 2.0 of RMG has a number of new features and enhancements. These include additional exchange-correlation functionals, including van der Waals interactions via VDW-df, a new multigrid-preconditioned Davidson-based eigensolver that offers better performance for small to medium-size systems, as well as general performance optimizations that typically reduce time to solution by a factor of 3 to 5 as compared to the previous version of RMG. Memory usage has been reduced and optimized, and additional density mixing algorithms have been added. The calculation of forces has been much improved, reaching similar levels of accuracy and speed as plane wave codes.

RMG is available for download from <https://sourceforge.net/projects/rmgdft>. Documentation, wiki, user forums, installation and getting started support are also provided. In addition to the source code, binary packages are supplied for the common Linux distributions, Macs and Windows. For the Cray systems, a portal for RMG has been established at <http://bluewaters.ncsa.illinois.edu/rmg>. Similar portals will be created for other major supercomputer sites and architectures.

An RMG tutorial will be presented during ES2016.

Electronic Structure Applied to Enzyme Decomposition Mechanism

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Bacterial type II L-Asparaginases (ASPII) have been used for over four decades to treat acute lymphoblastic leukemia, yet a full reaction mechanism remains unknown. ASPII enzymes catalyze the deamidation of both asparagine (Asn) and glutamine (Gln), which results in the formation of aspartate (Asp) and glutamate (Glu), respectively, and the by-product ammonia. Proposed ASPII mechanisms to date have yet to explain the absolute requirement of a substrate alpha-carboxyl group, and clearly identify the role of the catalytic threonines T12 and T89. Here, we study the reaction mechanism of asparagine degradation by ASPII through classical and *ab initio* molecular dynamics (MD) simulations as well as experiments [1-2].

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Correlation matrix renormalization method for studying correlated-electron materials

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We recently proposed a correlation matrix renormalization (CMR) theory to treat the electronic correlation effects [1, 2] in ground state total energy calculations of molecular and condensed systems using Gutzwiller variational wavefunction (GWF). The CMR method goes beyond the conventional Gutzwiller approximation and incorporates Coulomb interactions between two localized electrons on different atomic sites. By adopting a number of approximations, the computational effort of the CMR can be reduced to a level similar to Hartree-Fock calculations. In order to minimize the error originating from some of these approximations, we introduce a novel sum-rule correction to obtain a more accurate description of the inter-site electron correlation effects in total energy calculations. Benchmark calculations are performed on a set of molecules to show the reasonable accuracy of the method.

Work supported by US-DOE BES under Contract No. DE-AC02-07CH11358.

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Role of Hydrogen in the Electronic Properties of CaFeAsH-based Superconductors

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The electronic and magnetic properties of the new hydride superconductor CaFeAsH, which superconducts up to 47 K when electron-doped with La, and the isovalent alloy system CaFeAsH_{1-x}F_x are investigated using density functional based methods. The $\vec{Q} = (\pi, \pi, 0)$ peak of the nesting function $\xi(\vec{q})$ is found to be extremely strong and sharp, and we quantify additional structure in $\xi(\vec{q})$ associated with the near-circular Fermi surfaces (FSs) that may impact low energy excitations. We analyze the unusual band introduced by H, which shows strong dispersion perpendicular to the FeAs layers and is connected to a peculiar van Hove singularity just below the Fermi level. This band provides a three dimensional electron ellipsoid Fermi surface not present in other Fe-based superconducting materials nor in CaFeAsF. Electron doping by 25% La or Co has minor affect on this ellipsoid Fermi surface, but suppresses FS nesting strongly, consistent with the viewpoint that eliminating strong nesting and the associated magnetic order allows high T_c superconductivity to emerge. Various aspects of the isovalent alloy system CaFeAsH_{1-x}F_x and means of electron doping are discussed in terms of influence of incipient bands.

Evolution, Structure and Reactivity: Critical features for predicting As binding affinities in zinc finger proteins

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Arsenic is a known human carcinogen that can amplify the carcinogenicity of other DNA damaging agents such as UV radiation. One proposed mechanism for As carcinogenesis is the inhibition of DNA repair pathways through the disruption of the action of a class of proteins known as *zinc fingers*. This is caused by the displacement of the core Zn ions by As, leading to loss of zinc finger function and activity.

To understand this mechanism, we designed a molecular-based support vector machine (SVM) classifier that incorporates 12 features associated with evolutionary progression, protein structure before and after folding, and reactivity/structure in the vicinity of the metal binding region of the protein. Recent *in vitro* experiments have measured varying degrees of Zn loss for different sub-families of zinc finger proteins exposed to As. In order to map our initial binary SVM classifier predictions to the probability of Zn loss as measured in the laboratory, we have utilized the scaling methodology due to Platt [1]. As a first test of our approach, we restricted our feature set to two features known to be of particular importance from previous work: the number of Zn-coordinating cysteines [2] and $\Delta\Delta G$ relative binding energies (As vs. Zn) for each of the 22 zinc finger proteins studied [3]. $\Delta\Delta G$ values were computed for core Zn finger motifs (~54 atoms) at a high level of theory in Gaussian '09. Our results illustrate the ability of the mapped classifier to successfully model degree of Zn loss as observed in experiments. The additional features presented here will enable further refinement of Zn finger structural subclasses and their As binding affinities.

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Theoretical characterization of Hemibonds between X and HX (X=F, Cl, Br)

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Three-electron, two-center chemical bonds possess unusual bonding properties, such as a $\frac{1}{2}$ formal bond order and low but relevant bond energies. These so called “hemibonded” structures may impact reaction pathways, exercising stereodynamic forces that are important at low energies. For instance, hemibonded, pre-reaction complexes may have geometries that steer the complex towards a particular transition state. Recently, Douberly’s group reported[1] the trapping of a stable complex formed between Cl and HCl using He nanodroplet spectroscopy. Here we report our investigations of this complex and other halogen analogs using both Density Functional Theory (DFT) and Coupled Cluster (CC) with single, double, and triple excitations. Most of the calculations were carried out with the explicitly correlated, F12 version of the unrestricted coupled-cluster method with singles, doubles, and perturbative triples (CCSD(T)) based on restricted open-shell Hartree-Fock reference wave functions (ROHF-UCCSD(T)-F12a). F-HF, Cl-HCl, Br-HBr, F-HCl, Br-HCl were all examined to gain insight into related systems. Such systematic studies are necessary to establish trends in these complexes. Geometries, energies, and vibrational frequencies are reported for these complexes. Differences in DFT and CCSD(T)-F12 methods are discussed.

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Effects of Magnetization and Charge State in Hydrogen Dissociation over Copper Nanoclusters

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Heterogeneous transition metal catalysts play essential roles in the commercial production of platform chemicals, with popular examples including ammonia production on iron and methane steam reforming on nickel. The wide range of chemical and surface properties of transition metals, coupled with alloying and catalyst supports, already presents an enormous phase space for optimizing kinetics. However, recent improvements in synthesizing very small (1-2 nm or less) nanoclusters has revealed that quantum finite-size effects can dramatically affect binding and activation energies. The ability to control the specific structure and size of nanoclusters is therefore an exciting prospect, but to date a detailed understanding of how the electronic structure of nanoclusters affects catalytic performance is lacking. To help understand some of these effects in detail, we present recent results from a density functional theory study of hydrogen dissociation over Cu_{13} nanoclusters. We find the kinetics and reaction path are significantly different than those of the well-studied bulk Cu(111) surface, a direct result of the nanoclusters' strong finite size effects, especially their magnetization and charge states.

Ab-initio Study of Type II Semiconductor Superlattices within DFT+GW Formalism

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We report the recent stage of the ongoing study of type-II InAs/GaSb superlattices (SLs) within density functional theory (DFT) and correction of the screening of interaction by many body perturbative GW calculations. The effect of layer's thicknesses and the presence of interfacial layers on the electronic band gap and the semi-conductor to semi-metal transition of the SLs have been studied and compared with experimentally measured data for structures grown at our own lab. Although GW tends to correct the mean-field results, we observe that the final result does depend on the starting DFT calculations. The structures considered in this study are 8 monolayers (MLs) InAs / 8MLs GaSb and 10MLs InAs / 10MLs GaSb.

Perovskite to Post-Pervoskite Phase Boundary from Quantum Monte Carlo

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We have computed the free energies of (Mg,Fe)SiO₃ as functions of pressure, temperature, and composition, thus giving the equations of state and the Pv–PPv boundary^{1,2} using quantum Monte Carlo (QMC) simulations along with phonons from GGA+U density functional perturbation theory (DFPT) computations, which should rival experiment in accuracy. Our results agree well with the observations of the depth, thickness, and lateral variation of the D'' discontinuity, showing definitively that the D'' discontinuity is due to the PPv transition. Our QMC results also show the double crossing is possible in places where the iron concentration in (Mg,Fe)SiO₃ is no more than 13.5%, and have potential applications for modeling of Earth's whole mantle. We show that QMC is now robust and accurate for complex materials that contain transition metals, such as iron bearing Pv and PPv.

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Disorder in Organic Semiconductors Due to Fluctuations in Space Charge Density

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In organic semiconductors the charge mobility is many orders of magnitude lower than in inorganic counterparts due to weak (Van der Waals) molecular interactions and high energetic and spatial disorder. In many applications the density of injected charges is low, so that long-range Coulomb interactions between a moving charge with the static electric field set up by randomly oriented and randomly distributed permanent dipoles has been shown to lead to correlated Gaussian energetic disorder. However, another important source of static energetic disorder is the random field set up by permanently trapped (space) charge. Analytic models for which the energetic landscape has been calculated for randomly placed positive and negative charges have indicated anomalously large energy fluctuations, but this is because correlations between trapped charges have been largely ignored. In this work we introduce a mean-field model in which the dynamical correlations of the trapped charges can be calculated analytically. The model allows for a determination of the disordered electric field landscape set up by thermal fluctuations in the trapped charge distribution. We show that, in many systems of interest, charge transport will be thermally activated due to the energetic disorder caused by space charge fluctuations alone. Remarkably, in such a case, the activation energy depends only on the distance a charge hops, and is completely independent of the space charge density.

Aperiodic Weak Topological Superconductors

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Weak topological phases are usually described in terms of protection by the lattice translation symmetry. Their characterization explicitly relies on periodicity since weak invariants are expressed in terms of the momentum-space torus. We prove the compatibility of weak topological superconductors with aperiodic systems, such as quasicrystals.

We introduce a real-space formulation of the weak invariant, based on the Clifford pseudospectrum. A non-trivial value of this index implies a non-trivial bulk phase, which is robust against disorder and hosts localized zero-energy modes at the edge.

The Clifford pseudospectrum is similar to the local density of states. It is a scalar depending on location and energy. This scalar reflects the minimum possible variance in energy and position for an electron state with that expected value of energy and position.

100 meV gap Chern insulating phases achieved by design in transition metal buckled honeycomb lattices

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The discovery of quantum anomalous Hall (QAH) insulators, which was explained in terms of a bulk topological invariant known as the Chern number has attracted interest both as a novel electronic phase and for its anticipated applications in electronic devices. Honeycomb lattice systems such as we discuss here, formed by heavy transition-metal ions, have been proposed as topological insulators, but identifying a viable example has been limited by the complexity of the problem, appearing as an assortment of broken symmetry phases that must be studied and that sometimes thwart the topological character. The complexity has its positive aspect as well, providing many knobs to tune to obtain the desired properties. Here we use the flexibility of choice of spin-orbit and interaction strength, with tuning by strain, to design two buckled honeycomb Chern insulator systems with bandgaps up to 100 meV. Full structural relaxation is necessary, and the resulting lack of any symmetry whatsoever does not hamper the QAH character. Recent growth of insulating, magnetic phases in closely related materials supports the likelihood that synthesis and exploitation will follow.

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Ab initio study of M-doped BaSnO₃ (M= La, Y on A-site, Bi on B-site) using the ACBN0 Functional: Structural, Electronic and Optical Properties

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Using the recently developed pseudo-hybrid Hubbard density functional ACBN0 [1], we have studied the structural, electronic and optical properties of M-doped (M= La, Y on A-site, Bi on B-site) BaSnO₃. The study is motivated by recent experimental results which show that BaSnO₃ doped with Bi or La remains transparent for a wide range of dopant concentrations (up to 90 percent) and is a potential perovskite based transparent conducting material. Traditional DFT calculations on native BaSnO₃ and BaBiO₃ (LaSnO₃ is not a stable phase) fail to open the gap (both systems result as semi-metals), thereby hindering the study of doping in these materials. Using ACBN0 we demonstrate that the band gaps open and are in good agreement with experiments. In particular, in BaBiO₃, we correctly reproduce the crystal structure instability caused by the well-known breathing and tilting modes of the Oxygens, and the alternating ordering of Bi³⁺ and Bi⁵⁺ charges.

Simulations of the La-doped system indicate that experiments are not consistent with a random alloy model but can be interpreted invoking a structural ordering where BaSnO₃ and LaSnO₃ phase separate and are layered as a heterostructure. On the other hand, preliminary results on Bi doping show that the band gaps are significantly lower than in experiments if we assume a similar ordering. Further investigations on the structural details of the Bi-doped system are thus needed. Finally, we find that Y doping introduces shallow donor states close to the bottom of the conduction band while maintaining a large band gap, thus making the system another potential transparent conductor.

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Electronic structure contributions to molecular rectification

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Here we will explore two ongoing problems that are related to molecular rectification. The first study involves experimental and computational studies of donor-bridge-acceptor (D-B-A) biradical constitutional isomers (D: S=1/2 *ortho*-semiquinone, **SQ**; A: S=1/2 nitronynitroxide, **NN**) and the second study details our understanding of how a unique cofactor in Biology may be involved in promoting vectorial electron transfer.

The D-B-A biradicals effectively serve as constant bias analogs of molecular current rectifying devices. Biradical electronic couplings (H_{DA}) for asymmetric bridges (B = thiophene-pyridine, **T-P** and pyridine-thiophene, **P-T**) are described in terms of McConnell's electronic coupling theory and Nitzan's correlation between electronic coupling and conductance. Magnetic exchange couplings are used to estimate a rectification ratio (RR), yielding $g_{DTPA}/g_{DPTA} = 0.88$. Analysis of molecular conformations show that changes in the intrabridge torsion angle can change the sign of the RR. The small RRs inferred from this study result from electronic coupling being mediated by a highly symmetric **P-T/T-P** bridge LUMO, which promotes the electronic coupling in these biradicals. We will detail how the biradical approach can be used to derive key structure-property relationships that allow insight into the choice of bridge fragments for molecular rectification.

The active site of nearly all molybdoenzymes consists of a Mo ion coordinated by a redox active pyranopterin dithiolene ligand. Molybdoenzymes generally catalyze two-electron oxidation-reduction reactions that are coupled to atom transfer, with the active site being regenerated by two sequential electron transfer events. We have calculated the degree of molecular rectification mediated by the pyranopterin dithiolene as a means of assessing its putative role as an electron transfer conduit. We compute a large rectification ratio of ~3.4 at a bias of +0.4. We have also evaluated the nature of the eigenchannels used by the pyranopterin dithiolene to determine orbital contributions to the electron transfer reactivity mediated by this unique cofactor ligand in biology.

Phase Stability of TiO₂ Polymorphs from Diffusion Monte Carlo

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Transition metal oxides (TMO) are versatile compounds with a number of actual and potential applications because of their coupling between charges, spin, and lattice degrees of freedom [1]. Titanium dioxide, TiO₂, is a particular 3d transition metal oxide of great interest because of its multiple applications in catalysis, energy conversion and memristive devices due to its electronic structure [2]. Most of applications utilize the naturally existing phases: rutile, anatase and brookite. In spite of the simple form of TiO₂ and its wide uses, there is long-standing disagreement between theory and experiment on the energetic ordering of these phases that has never been resolved [3]. We present the first analysis of phase stability at zero temperature using the highly accurate fixed node diffusion Monte Carlo (FN-DMC) method. We also study the temperature effect by calculating the Helmholtz free energy including both internal energy corrected by DMC and vibrational contribution from phonon calculations with quasi harmonic approximation (QHA) via density functional perturbation theory (DFPT). We show that the effect of lattice vibration caused by finite temperature is crucial to the relative stability between these phases.

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Modeling Charge Transfer Gaps and Their Closure at the Atomistic Scale

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We develop an atomistic-scale model Hamiltonian that allows for charge transfer among sites or atoms in a system through a charge-transfer hopping mechanism, rather than through chemical potential equilibration alone [1]. From the energies for the different charge states of a system, one can calculate chemical potentials for adding (μ^+) and removing (μ^-) an electron from the system. This evaluation corresponds to systems at "half-filling" in more traditional approaches to problems of gap closure [2]. The charge transfer gap $\Delta\mu$ is the difference between μ^+ and μ^- [3]. Because a hopping mechanism is retained explicitly in the model, electron (T^+) and hole (T^-) hopping can reduce the charge transfer gap of the atoms (U) comprising the system. For simple ring systems with only nearest-neighbor hopping, expressions for $\Delta\mu$ can be derived analytically to find

$$\Delta\mu = U - |T^+| - |T^-| .$$

This is the expected result, but derived from model Hamiltonians at the atomistic scale, not the electronic-structure scale. There is no explicit spatial dimensionality dependence in any of the energies. U is comparable in meaning to the Hubbard U , Parr-Pearson hardness η , and Mott exciton pair-formation energy ϵ_M . The results are contrasted with those from more traditional electronic structure approaches, such as Hubbard and Gutzwiller models.

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Joint Density-Functional Theory Investigations of Atomic-Scale Structure and Energetics at the Solid-Liquid Interface

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Understanding the complex and inherently multi-scale interface between a charged electrode surface and a fluid electrolyte would inform design of more efficient and less costly electrochemical energy storage and conversion devices. Joint density-functional theory (JDFT) [1] bridges the relevant length-scales by joining a fully *ab initio* description of the electrode with a highly efficient, yet atomically detailed classical DFT description [2] of the liquid electrolyte structure, avoiding the costly statistical sampling of the liquid required by molecular dynamics calculations. Leveraging JDFT within our framework to treat charged systems in periodic boundary conditions [3] we then predict the voltage-dependent structure and energetics at the interface between a liquid electrolyte and graphitic, single-crystalline metallic, and complex oxide electrodes. We compare the JDFT-predicted interfacial water structure next to a graphitic electrode with results obtained from classical and *ab initio* molecular dynamics simulations. We go on to elucidate the physical origin of the experimentally measured voltage-dependent differential capacitance of an Ag(111) electrode in aqueous NaF electrolyte, examining the crucial role of ion desolvation and plating onto the electrolyte. Finally, we conclude with an exploration of how the surface structure of a LiMn₂O₄ electrode [4] changes in the presence of a liquid battery electrolyte and as a function of applied potential.

Use of the Center for Nanoscale Materials, an Office of Science user facility, was supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

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Poster Abstracts II
Tuesday Session

(number indicates poster location)

Hydrogen mediated sulfur defect healing in a monolayer MoS₂

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The molybdenum disulfide (MoS₂) has a layered structure, from which a monolayer MoS₂ can be exfoliated. In mechanically exfoliated MoS₂, a certain amount of defects and impurities are always present, and even with the small imperfections, their electrical and optical properties are largely affected. Most defects in a monolayer MoS₂ generate deep defect states in the band gap, which act as electrons/hole trap centers. This leads bad optical and electrical properties. The low photoluminescence (PL) intensity of the monolayer MoS₂ may come from naturally existing defect recombination centers such as S-vacancy generating the deep defect states in the band gap. The S-vacancy acts as the electron capturing center, thus it should be healed to enhance the properties of MoS₂. Recently, Amani *et al.* have found that, by the superacid treatment using TFSI, the PL quantum efficiency in the monolayer MoS₂ has enhanced, and the Mo/S ratio has increased indicating the reduction of S-vacancy. [1] In this work, we carry out the first-principles calculations to investigate the S-vacancy reducing mechanism on a monolayer MoS₂ in hydrogen rich environment. To understanding healing mechanism of the S-vacancy on a monolayer MoS₂, we calculated the reaction energies of a systems mediated by the hydrogen. Although the migration of sulfur defects is impossible by itself, the hydrogen extremely rich environment can reduce the S-defects on a MoS₂ surface to be clean.

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The Defect Band Gap

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The Kohn-Sham (KS) band gap in density functional theory (DFT) is typically (much) smaller than the experimental band gap for semiconductors, the infamous “band gap problem” of DFT. It is often asserted that a bad KS band gap makes it impossible to compute accurate defect levels in semiconductors—the band gap defines the energy scale for the defect levels, after all. This assertion is shown to be false, using the results of comprehensive defect studies in multiple materials using standard semilocal LDA and PBE functionals that express a band gap problem. In Si and GaAs the computed defect levels match experiment to ~ 0.1 eV. Moreover, the “defect band gap”, defined as the span of valid defect levels computed from total energy differences, applying rigorous and self-consistent control charge boundary conditions in fully size converged supercell calculations, proves to yield accurate predictions of the band gap. Computed defect band gaps for several other III-V, II-VI, IV-IV semiconductors and other compounds also agree with the experimental band gap. Where is the band gap problem? What is the band gap problem? Current understanding of what the “band gap problem” means—and how to “fix” it—needs to be rethought.

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Photoinitiated electronic relaxation processes

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As the realization for renewable energy sources has come to the forefront, developing materials and understanding processes to increase the efficiency of solar energy harvesting has been a goal of many researchers. Two possible approaches to produce high photovoltaic device efficiencies are chemical composition and device architecture of photoactive materials. Methylammonium lead iodide perovskite (MAPbI₃) materials have been successfully applied in photovoltaic devices providing high solar energy conversion efficiencies, driving researchers to find the fundamentals of the material's behavior. Physical modifications, such as quantum confinement, have also shown to improve optoelectronic properties and solar energy conversion efficiencies in a multiple semiconducting materials. Here we provide a computational approach to studying radiative (R), non-radiative (NR), non-radiative recombination (NRR), and multi-exciton generation (MEG) electronic transition processes within a spatially confined MAPbI₃ quantum dot (QD). Understanding electronic transition pathways and their corresponding timescales in such nanostructures allows for a clearer view into which relaxation processes are of greatest importance and which will maximize charge collection efficiency. Relaxation rates for NR and NRR processes are calculated by nonadiabatic dynamics and density matrix formalism producing rates on the timescale of 1ps. Relaxation rates for R processes, computed by estimating oscillator strengths in the independent orbital approximation, are on the timescale of 10ps. Relaxation rates for MEG processes are computed with many-body perturbation theory and found to be on the time scale of 10fs. From the computed relaxation rates, the mechanism timescales trend in the order of MEG > NR > R > NRR. From these results one expects that quantum confinement makes MEG a highly probable relaxation pathway in a MAPbI₃ QD. The rates of NR relaxation within the MAPbI₃ QD are also compared to 3D bulk MAPbI₃ materials, showing a decreased NR and R relaxation rate due to the effects of size confinement.

Understanding molecular interactions with metal surfaces: The case of HCl on Au(111)

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Understanding the interaction of molecular species with metal surfaces has profound implications in many areas, including heterogeneous catalysis, corrosion prevention, and energy production. Although general properties of these interactions are relatively easy to study experimentally, theory is often required for a more detailed understanding. Indeed, theoretical approaches have yielded great insight into how molecules interact with surfaces in a number of important cases. Despite this, some of the most interesting cases are difficult to study computationally, either because of the large time or length scales required, or because significant non-adiabatic effects confound the usual approximations. Generally speaking, an energetic molecule impinging on a metal surface can either react (often via dissociative adsorption) or scatter from the surface. In the case of HCl on a Au(111) surface, both of these processes exhibit interesting behavior that is not yet fully understood, making this an ideal system for detailed computational study. This work seeks to combine several state-of-the-art computational approaches, including ab initio molecular dynamics, atomistic neural network potentials, and friction models of electron-hole pair effects, to further the understanding of the fundamental processes affecting the interaction of HCl with a Au(111) surface.

Phonon-mediated superconductivity and related phenomena in two-dimensional boron

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Flat monoelemental boron is a metallic 2D solid predicted to have a number of intriguing properties. The calculated electron-phonon coupling in this material is large enough [1] for it to possibly be a conventional superconductor with $T_c \sim 10\text{-}20$ K, assuming the value $\mu^* = 0.1$ for the Coulomb pseudopotential. However, this bulk-optimized μ^* value may not be applicable in 2D systems. Since, unlike bulk systems, experimental measurements of T_c are scarce in 2D, having a predictive theory, such as the ab initio theory of superconductivity [2], is of paramount importance. In this work, we consider two-dimensional boron as a model system (and already a reality [3]) to study superconductivity as well as other related many-body phenomena in two-dimensional solids. Calculated electron and phonon spectra of 2D boron polymorphs show rich features that, beyond superconductivity, point at the possibility of existence of Kohn anomalies, charge density waves, and Peierls instabilities in this material. We thus show this material to be a great testbed for new first-principle approaches to many-body phenomena in 2D systems.

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First-principles prediction of a stable hexagonal phase of $\text{CH}_3\text{NH}_3\text{PbI}_3$

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Methylammonium lead iodide (MAPbI_3) is a promising new photovoltaic material with high power conversion efficiency. We have used first-principles density functional theory calculations to study the stability and optoelectronic properties of different polymorphs of MAPbI_3 under volumetric and epitaxial strain. We predict a novel hexagonal (*H*) phase of MAPbI_3 with $P6_3/mmc$ space group to be thermodynamically the most stable phase among all observed phases of MAPbI_3 . The *H*-phase consists of alternating layers of face-shared PbI_6 octahedra and organic MA cations, which is in contrast to the corner connectivity of the octahedra observed in the experimentally reported orthorhombic (*O*), tetragonal (*T*), and cubic (*C*) phases of MAPbI_3 . The change in octahedral connectivity leads to large changes in the band structure and optoelectronic properties. The *H*-phase has an indirect band gap of 2.6 eV, which is ~1.2 eV larger than the direct band gap of *T*-phase. The stability of the different polymorphs using different exchange-correlation functionals, dispersion-forces and spin-orbit coupling effects will be presented. Finally, the effect of volumetric and epitaxial strain to tune the band gap of MAPbI_3 by stabilizing the different polymorphs will be discussed.

Numerical Computations of the Pseudospectrum for the Chern Hamiltonian on a the Thin Film 2-D Hall Bar Geometry

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A Chern Insulator film [1] in the shape of a Quantum Hall Bar is used to demonstrate the topological phases in the bulk and at the edge as a function of bridge and contact dimensions in the presence of disorder. Electrons are localized near the boundary and at approximately zero Fermi energy creating the “edge effect.” The goal is to quantify the stability of the system in the presence of disorder. The topological phases are depicted based upon the pseudo-spectrum of the system [2]. Symmetry classes other than the Chern insulator class may also be considered for other geometries.

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Modeling Pseudo-Magnetic Field in Large Graphene Structures

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In this work we study the phenomenon of strain induced pseudo-magnetic field in graphene. The Hamiltonian for graphene near K, K' valleys is similar to that of the massless Dirac equation or, the Weyl equation. While under strain, the electronic hopping parameters among carbon atom sites are perturbed, which can be translated into an effective gauge field \mathbf{A} in the Hamiltonian:

$$H = v_F \boldsymbol{\sigma} \cdot (\hat{\mathbf{p}} \pm \mathbf{A})$$

By choosing the proper strain pattern, one can mimick the effect of a strong magnetic field, quantizing the band structure into pseudo-Landau levels. Application of a certain strain pattern produces the desired pseudo-magnetic field, but also destroys the translational symmetry of the graphene lattice, making Bloch theorem no longer applicable. Therefore the direct diagonalization of the full Hamiltonian, scaling as $O(N^3)$, becomes necessary, which is computationally prohibitive. One way to tackle this problem is to note that the pseudo-Landau levels of interest fall around the Fermi level. Using implementation² of the spectrum slicing algorithm, we can solve for only the subset of eigenvalues around the Fermi level, leading to large improvement in speed. Another way is to consider additional symmetry in the strained graphene structure. Certain desirable strain patterns can be realized in helically (twisted graphene ribbons³) or rotationally (graphene ribbon rings) symmetric structures. With these new symmetries taken into account, the Hamiltonian matrix becomes circulant, requiring only $O(N)$ computational cost.

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Ligand Control of Donor-Acceptor Excited-State Lifetimes

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We have synthesized a series of square-planar (dichalcogenolene)Pt(diimine) complexes and studied their excited state properties using a combination of transient absorption spectroscopy, emission spectroscopy, and electronic structural computations. The spectroscopic studies reveal charge-separated dichalcogenolene \rightarrow diimine charge-transfer excited state lifetimes that do not display a periodic dependence on the heteroatoms, E, of the dichalcogenolene ligand. We explain these results in terms of metal and ligand spin-orbit coupling, E-dependent singlet-triplet (S-T) energy gaps, and anisotropic covalency contributions to the M-E (E = O, S, Se) bonding scheme with the aid of electronic structural computations and group theory. For the dioxolene complex, 1-O,O, we find that $E(T_2) > E(S_1)$ and this leads to rapid nonradiative decay between S_1 and S_0 . In marked contrast, for the heavy atom congeners $E(T_2) \leq E(S_1)$ providing a mechanism for rapid intersystem crossing. Subsequent internal conversion to T_1 produces a long-lived, emissive triplet. The three LPtL' complexes with mixed chalcogen donors and 6-Se,Se display excited state lifetimes that are intermediate between those of 1-O,O and 4-S,S.

Keywords: Electronic Structure, Spin-Orbit Coupling, Charge Transfer, Donor-Acceptor, Excited State

Efficient and accurate GW calculations for 2D semiconductors using exact limits for the screened potential: Band gaps of MoS₂, hBN, and phosphorene

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Calculating the quasiparticle (QP) band structure of two-dimensional (2D) materials within the GW self-energy approximation has proven to be a rather demanding computational task. The main reason is the strong \mathbf{q} -dependence of the 2D dielectric function around $\mathbf{q} = \mathbf{0}$ that calls for a much denser sampling of the Brillouin zone than is necessary for similar 3D solids. Here we use an analytical expression for the small \mathbf{q} -limit of the 2D response function to perform the BZ integral over the critical region around $\mathbf{q} = \mathbf{0}$. This drastically reduces the requirements on the \mathbf{q} -point mesh and implies a significant computational speed-up. For example, in the case of monolayer MoS₂, convergence of the G₀W₀ band gap to within 0.1 eV is achieved with 6×6 \mathbf{q} -points rather than the 36×36 mesh required with discrete BZ sampling techniques. We perform a critical assessment of the band gap of the three prototypical 2D semiconductors MoS₂, hBN, and phosphorene including the effect of self-consistency at the GW₀ level. This method is implemented in the open source GPAW code[1].

[1] <https://wiki.fysik.dtu.dk/gpaw/>

First-principles study of sulfur atom doping and adsorption on α -Fe₂O₃ (0001) film

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Abstract

Using the spin-polarized density functional theory (DFT) and the DFT + U method, the geometric and electronic properties of the sulfur (S) atom doping and adsorption with the hematite α -Fe₂O₃ (0001) film have been investigated systematically. The most stable hematite α -Fe₂O₃ (0001) film with an anti-ferromagnetic arrangement is identified. For the study of sulfur adsorption on the film, the S adatom prefers to bond with three O atoms, in the center of a triangle formed by the three O atoms. The S acts as a cation at this site. The sulfur adsorption has introduced a couple of gap states, in addition to the unoccupied surface states. Furthermore, with the most stable S-adsorption configuration, the diffusion of the S adatom from the surface to the inside is searched and the transition state along the minimum-energy pathway is also evaluated. For S-doping in the film, it is found that S substitution of O in the top layer is energetically favoured than that in the deeper layer. It shows that the value of the band gap is reduced to $\sim 1.26\text{eV}$ from $\sim 1.43\text{eV}$ of the clean film. The formation energy of S substitution of O in the film is also obtained.

Interlayer Binding of Bilayer Low-dimensional sp -, sp^2 -Hybridized Carbon Networks : Quantum Monte Carlo Study

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We have used Quantum Monte Carlo (QMC) methods to study the interlayer binding of an α -graphyne bilayer. Theoretical quantitative measurements of van der Waals (vdW) interactions between low dimensional carbon allotropes were usually carried using Density Functional Theory (DFT) with a limited success. In a recent study, QMC methods were used to describe accurately interlayer binding energies of a bilayer graphene. Results also showed that vdW-corrected DFT functionals tend to overestimate interlayer bonding nature of a sp^2 -bonded carbon network. [1] More recently, sp -, sp^2 - hybridized α -graphyne have been the subject of many studies due to its different and unique electronic properties compared to the graphene's. Previous DFT calculations on bilayer α -graphyne predicted two energetically stable stacking modes (Ab and AB) among six possible modes, and split gaps in the Ab mode tunable with an external electric field normal to the surface. However, since determining the most stable mode within the DFT framework is strongly dependent on the vdW-correction scheme applied to the exchange and correlation functional, the most stable mode for the bilayer α -graphyne couldn't be confirmed. [2]

In this study, QMC calculations confirmed that an AB stacking mode is the most stable (by 0.9(3) meV/atom) compared to the Ab mode. In addition, we found that vdW-corrected DFT binding energies significantly underestimate interlayer bindings of sp -, sp^2 - hybridized carbon network systems while overestimate sp^2 - bonded graphene.

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**Coupling quantum Monte Carlo and independent-particle calculations:
self-consistent constraint for the sign problem
based on density and density matrix**

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The vast majority of quantum Monte Carlo (QMC) calculations in interacting fermion systems require a constraint to control the sign problem. The constraints involve an input trial wave function from external calculations. We introduce a systematically improvable constraint which relies on the fundamental role of the density or one-body density matrix. An independent-particle calculation is coupled to an auxiliary-field QMC calculation. The solution from the independent-particle calculation is used as the constraint in QMC, which then produces the input density or density matrix for the next iteration of the independent-particle calculation. The process is iterated until self-consistency is reached.

The method provides an optimized constraint which improves the accuracy and predictive power of QMC. Conversely, it enables independent-particle calculations with better densities or density matrix. Our approach also provides an *ab initio* way to predict effective “ U ” parameters for independent-particle calculations. We demonstrate the method in a prototypical strongly correlated system, the doped two-dimension Hubbard model, by accurately determining the spin densities when collective modes are present in the magnetic and charge correlation which are separated by tiny energy scales.

Fragment Approach to Density Functional Theory Calculations of Large Systems

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Density-functional theory (DFT) has become the dominant method for electronic structure simulations due to its excellent balance between accuracy and efficiency. However, standard implementations of DFT scale cubically with the number of atoms and so reduced scaling algorithms are required to allow simulations of realistic (large) systems of technological importance. To this end, a linear-scaling approach has recently been implemented in BIGDFT, wherein a minimal set of localized support functions are expressed in an underlying wavelet basis and optimized to reflect their chemical environment¹. This not only allows the treatment of tens of thousands of atoms, but also facilitates the straightforward definition of a fragment approach, which reduces the computational cost by up to an order of magnitude while also offering additional flexibility. Such an approach has previously been applied to supramolecular systems, where it was shown to be effective in treating environmental effects within the context of constrained DFT². An embedded fragment approach has also now been developed for extended systems, which is particularly suited to the treatment of defective materials. We will describe the BIGDFT fragment approach and present examples of its application to both molecular and extended systems.

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Recent Developments in TDDFT of Warm Dense Matter

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Warm dense matter (WDM) is matter at the edge of chemical stability, due to intense pressures and temperatures. As the conditions are intermediate between a condensed phase and an ideal plasma, WDM presents a unique theoretical challenges that requires borrowing ideas from plasma physics and quantum chemistry. Even so, standard wave function methods from quantum chemistry become cost prohibitive, as systems of interested are best treated as extended, and the elevated temperatures require the inclusion of many virtual states. Motivated by the established success of DFT-MD in characterizing the thermodynamic properties of WDM, we have implemented finite temperature time-dependent density functional theory (TDDFT) to compute a number of quantities of relevance to high pressure research, including optical conductivity, stopping power, and the dynamic structure factor. We will provide details of our framework and focus on recent results in which we have performed the first calculations of the dynamic structure factor of shock-compressed beryllium independent of the widely used Chihara model [1]. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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Electron-phonon coupling beyond semilocal DFT

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Electron-phonon coupling is ubiquitous in condensed matter, and plays central roles in superconductivity, transport, and the temperature dependence of optical properties. First-principles calculations of electron-phonon coupling are almost exclusively performed using semilocal density functionals, but it has been recently shown that electronic correlations can have a large effect. Unfortunately, electron-phonon coupling beyond semilocal DFT remains a computationally challenging task.

We propose two novel approaches to the finite difference calculation of electron-phonon coupling that enable the routine use of methods beyond semilocal DFT. The first development concerns the use of nondiagonal supercells to reduce the scaling of supercell sizes from cubic to linear.¹ The second development uses the mean value theorem for integrals to select a special atomic configuration that captures the full strength of electron-phonon coupling with a single or very few calculations.²

We apply the proposed methods in two studies. In the first, we use the *GW* approximation to calculate the electron-phonon coupling induced temperature dependence of the band gaps of a range of standard semiconductors and insulators.³ We find that electronic correlations must be included to match experiment. In the second, we use semilocal and hybrid functionals with spin-orbit coupling to study temperature-induced band inversions in topological insulators. We find that in the Bi_2Se_3 family of compounds, increasing temperature favours the trivial phase over the topological phase.

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Polaron-induced phonon stiffening in rutile TiO_2

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Crystalline transition metal oxides such as TiO_2 , NiO , CoO possess attractive properties for photo-catalytic, photo-voltaic and other applications. Despite several decades of research, carrier-ion interactions that account for many important properties of these materials, such as carrier mobility and effective mass, are still the subject of controversy. Here we study fundamental polaron properties in rutile TiO_2 both experimentally, using Raman spectroscopy of photo-excited samples, and computationally, with the real-time time-dependent density functional theory (RT-TDDFT) mixed quantum-classical method, which employs mean-field classical (Ehrenfest) dynamics to couple the electronic and ionic subsystems. In both experiment and theory we observe an unexpected stiffening of the A_{1g} phonon mode under UV illumination. We computationally analyze the polaron structure and provide an explanation for the stiffening. We find that small polaron formation in rutile titania is a strongly non-adiabatic process and that Ehrenfest classical-ion dynamics is an adequate method to describe its dynamics and time scales.

Topological nature of alkaline earth-pnictide compounds with antiperovskite structure

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Searching for new topological insulators, especially those that may have useful applications of their charge or spin conducting surface bands, is a current research priority. In three dimensions (3D), topological insulators are characterized by a Z_2 index, and have gapless edge states providing a quantum spin Hall character. Z_2 strong and weak topological insulators are distinguished from a normal insulator by four independent Z_2 invariants $\nu_0(\nu_1\nu_2\nu_3)$. Sun and collaborators¹ have noted that cubic antiperovskite compounds (viz. Ca_3BiN , with N in the octahedron of Ca ions) can become TIs with applied (001) strain. Here we survey the entire class ($3 \times 5 \times 5$ compounds) of alkaline earth - pnictide antiperovskite compounds, viz. $\text{X}_3\text{PnPn}'$, where $\text{X} = \text{Ca, Sr, Ba}$ is an alkaline earth element and $\text{Pn, Pn}' = \text{N, P, As, Sb, Bi}$ are pnictide elements, using density functional methods. Due to their inversion symmetry, the Z_2 topological invariants can be determined from the parity of the occupied bands at the time-reversal invariant momenta (TRIMs). Results show that spin-orbit coupling and strain are important to the topological nature of AE-Pn antiperovskite compounds. While some compounds (mainly those with nitrogen inside the octahedron, e.g. Ca_3BiN) need both spin-orbit coupling and proper strain to have band ordering inverted, some (e.g. Ca_3BiP) only need spin-orbit coupling to induce the band inversion, giving a Z_2 invariants of 1(000), but with valence band maximum and conduction band minimum touching at Γ point, producing a topological semimetal state, whereupon strain will produce a transition to topological insulator. The energetic stability and the band structure characteristics of the antiperovskite compounds will be addressed, and a case study of Ca_3BiP will be presented, including the effect of strain that can transform the topological semimetal into topological insulator, producing the topologically protected surface state.

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Developing Highly Scalable GW Calculations Within the OpenAtom Software

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Designing novel materials such as new photovoltaics, optical devices, and catalysts require a proper description of electronically excited states. In terms of *ab initio* methods, the GW and Bethe-Salpeter Equation (GW-BSE) beyond DFT methods have proved successful in describing electronic excitations in many materials. However, the heavy computational loads and large memory requirements have hindered their routine applicability by the materials physics community.

We outline some of our collaborative efforts to develop a new parallel software framework designed for GW calculations on massively parallel supercomputers. Our GW code is interfaced with the plane-wave pseudopotential *ab initio* molecular dynamics software “OpenAtom” [1] which is based on the Charm++ parallel library [2, 3]. The computation of the electronic polarizability is one of the most expensive parts of any GW calculation. To avoid the large number of fast Fourier transforms (FFTs) common to most GW methods, we employ a real-space representation when computing the electronic polarizability matrix. We describe parallel scaling results for the polarizability calculation up to thousands of nodes (tens of thousands of cores). We also describe our work on implementing the static (so called “COHSEX”) GW self-energy. The advantages of such a real-space approach for quasi-particle calculations will be outlined.

This work is supported by National Science Foundation through grant ACI-1339804.

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Magnetic properties and exchange interactions in transition metal oxides: Benchmarking the ACBN0 functional

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We study the magnetic properties and magnetic exchange interactions in the $3d$ transition metal (TM= Mn, Co, Fe and Ni) oxides using the recently developed ACBN0 functional which is a parameter-free extension of traditional DFT+U functional where the Hubbard U is calculated self-consistently and depends on the electron density of the system. We show that ACBN0 greatly improves the electronic properties of the TMOs by improving the band-gap in MnO and NiO and making CoO and FeO insulating which is otherwise described incorrectly within DFT (LDA/GGA) functionals. The magnetic properties (magnetic moments, magnetic ordering energies, exchange coupling constants (J 's)) are all better described by ACBN0 at par with the Hybrid functionals and in closer agreement with the experimental values. For MnO and NiO, we investigated the magnetic properties at equilibrium and under pressure and found a good agreement with other advanced functionals. For all the oxides studied here, we did a thorough and extensive study by comparing different pseudopotentials and find overall that ACBN0-LDA is better for describing magnetic properties compared to ACBN0-PBE. We also discuss the application of ACBN0 to two multi-valent systems Mn_3O_4 and Co_3O_4 , where it is possible to evaluate U for different sites and different chemical bonding.

Calculation of observables and correlation functions from auxiliary-field quantum Monte Carlo

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The quantitative study of correlated materials requires accurate calculations of electronic density, forces and correlation functions.

To achieve this goal, we have formulated and implemented a back-propagation scheme [1] in the auxiliary-field quantum Monte Carlo [2].

The numerical stability and computational complexity of the technique are discussed, and its accuracy is assessed computing ground-state properties for small and medium-sized molecules. Applications for solids using plane-wave bases are also discussed.

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Probing (110) Facet of Rutile-Like ZnF₂ with CO: A DFT Study

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Adsorption of gaseous particles on solids offers a broad array of idiosyncratic functional properties such as those observed in scattering experiments. Nowadays, it is well-entrenched that physisorption acts as a precursor paving the way of chemisorption and the subsequent catalytic processes. Adsorption of small particles such as CO onto crystalline surfaces epitomizes physisorption. Due to its intricate nature, a delineation of the physical adsorption phenomenon is necessitated. This has incentivized a vast number of studies centered around the fundamental aspects of adsorption. The physical adsorption onto insulating surfaces with rutile-like structures was investigated using dispersion free and dispersion-corrected density functional theory. PBE and optB88-vdW were employed alongside plane-wave basis sets to carry out the calculations. Surface energies and atomic displacements with respect to bulk-terminated structure were computed for (110) plane of rutile-ZnF₂. For the first time, physisorption of CO on the aforementioned surface was modelled for monomer and monolayer sorption. The obtained values were in reasonable agreement with the pertinent literature when available.

Bethe-Salpeter Equation Calculations of Color Center Defects in Diamond

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Colored diamonds are of fundamental, technological, and commercial interest. The origin of their colors has long been the focus of both theoretical and experimental studies. For example, experiments have found that the color of blue diamonds is associated with isolated boron impurities,¹ while nitrogen impurities are responsible for yellow and pink diamonds. It has also been found that theoretical Bethe-Salpeter Equation (BSE) simulations of boron-doped diamonds yield optical absorption spectra in good agreement with observations.² In contrast, the nature of the nitrogen defects is less well understood, due to a plethora of possible N-defect configurations. Here we present a theoretical study of the optical spectra of nitrogen-doped diamonds that combines *ab initio* DFT calculations of structure with BSE calculations of the spectra from various N-defect conformations. In particular, we treat N_xV_y defect sites, where x is the number of substitutional nitrogen atoms and y is the number of carbon vacancies within relaxed 64-atom unit cells. Our calculations suggest that among the seven defect configurations studied, the most likely candidates for yellow-colored diamonds have N_2V_0 and N_2V_1 defects, while N_1V_1 defects are likely candidates for pink-colored diamonds.

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[*] This work was supported by DOE Grant DE-FG03-45623 (JJK, JJR) and NSF REU Grant PHY-1262811 (WHL).

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