CCP2018

XXX IUPAP Conference on Computational Physics
July 29 – August 3
University of California, Davis, USA

Abstracts / Parallel Sessions

CONTENTS

Monday, Parallel Sessions 1, 02:00PM-03:30PM

Machine Learning 1

Conference Center, Ballroom A

Invited: Artificial intelligence: a new tool for the study of quantum many-body systems

Ehsan Khatami
San Jose State University, San Jose, USA

Machine learning techniques have found their way into the field of quantum many-body physics in recent years and have emerged as promising new tools in our numerical toolbox for representing quantum states of matter or identifying phases and phase boundaries for models with critical or topological behavior among other things. In this talk, I will focus on supervised learning with artificial neural networks and how they can be used to identify magnetic phase transitions in the Fermi-Hubbard model or accelerate quantum Monte Carlo simulations. I will demonstrate how we can find out, to some extent, what the machines learn and how those information can lead us to new physics. I will also discuss the potential for clustering and other dimension-reduction methods to provide insight into the critical behavior of quantum many-body models.

K. Ch'ng, J. Carrasquilla, R. G. Melko, and E. Khatami, Phys. Rev. X 7, 031038 (2017); K. Ch'ng, N Vazquez, and E. Khatami, Phys. Rev. E 97, 013306 (2018)

Regression-based clustering for material analysis

Duong-Nguyen Nguyen[1], Tien-Lam Pham[1,2], Viet-Cuong Nguyen[3], Hieu-Chi Dam[1,4,5]
[1]Japan Advanced Institute of Science and Technology, 1-1, Asahidai, Nomi, Ishikawa, 923-1292, Japan. [2]ESICMM, National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan. [3]HPC Systems Inc., Tokyo, Japan. [4]Center for Materials Research by Information Integration, National Institute for Materials Science 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan. [5]JST, PRESTO, 4-1-8 Honcho, Kawaguchi, Saitama, 332-0012, Japan

In the present work, we propose the flow of data analysis for the extraction of the grouping of materials with similar characteristics; subsequently, the obtained information can be utilized to understand the data set and to construct a model capable of predicting the physical properties of materials. The data analysis flow consists of three steps: variable selection based on non-linear regression, regression-based clustering, and cluster interpretation by a decision tree. Several data sets of well-characterized crystalline compounds represented using fundamental atomic descriptors are used as test beds. The formation energy, lattice parameter, and Currie temperature are considered as target physical properties of the examined materials. Based on the information obtained regarding the group of materials, decision trees are constructed to interpret the cluster structure of the materials, and mixed regression models are constructed to estimate the physical properties of the materials. Our experiments show that rational and meaningful group structures can be obtained, and the proposed mixed model significantly improves the accuracy of the prediction of physical properties of materials.

ChIMES: Machine-Learned Force Fields for Quantum-Accurate Reactive Simulation

Rebecca Lindsey[1], Nir Goldman[1,2], Sorin Bastea[1], Laurence Fried[1]
[1]Lawrence Livermore National Laboratory, Livermore, USA. [2]University of California, Davis, USA

Understanding chemistry at extreme conditions is crucial in fields including geochemistry, astrobiology, and alternative energy. First principles (quantum-mechanical) methods can provide valuable microscopic insights into such systems while circumventing the risks of physical experiments, however the time and length scales associated with chemistry at extreme conditions (ns and μm, respectively) largely preclude extension of such models to molecular dynamics. In this work, we develop ChIMES, a generalized *n*-body force field comprised of linear combinations of Chebyshev polynomials that retains the accuracy of quantum-mechanical (QM) methods while decreasing computational effort by several orders of magnitude. Models are rapidly generated by mapping to forces arising from short density functional theory (DFT) trajectories through standard linear fitting approaches and refined self-consistently. We present development and application of ChIMES toward modeling molten carbon and understanding reactive nucleation of carbon condensates, and briefly discuss current challenges in extension of ChIMES to increasingly complex systems.

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. LLNL-ABS-751889

Advances in machine learned potentials for molecular dynamics simulation

Kipton Barros, Justin S. Smith, Nicholas Lubbers
Los Alamos National Lab, Los Alamos, USA

Recent breakthroughs in machine learning allow us to emulate quantum physics with stunning fidelity. For example, the latest deep neural networks can predict molecular properties with accuracy comparable to density functional theory, and approaching that of coupled cluster theory, at a tiny fraction of the computational cost. We present methods for building machine learned potentials that will enable large-scale and highly accurate molecular dynamics simulations, e.g., for chemistry, materials science, and biophysics applications. Key ideas are:

1. *Encoding known physical properties* and symmetries in the neural network architecture.
2. *Active learning* to dynamically augment the training dataset with new quantum calculations in regions where the machine learned model is uncertain.
3. *Transfer learning*, such that we first train on a large quantity of relatively low-fidelity data, and then perform some final training iterations using a smaller quantity of high-fidelity data.

Materials 1

Conference Center, Ballroom B

Invited: Extending the Scale with Real-Space Methods for the Electronic Structure Problem

James Chelikowsky
University of Texas, Austin, USA

In principle, the electronic structure of a material can be determined by a solution of the many-body Schrödinger equation. This was first noted by Dirac shortly after the invention of quantum mechanics in 1929. However, Dirac also noted that that the solution of the many body quantum mechanical equations were much to difficult to be solved. He challenged his colleagues to develop "approximate practical methods of applying quantum mechanics..."

Two key physical practical concepts have been developed to address Dirac's challenge: pseudopotential theory and density functional theory. For weakly correlated systems, this formalism works well for ground state properties such as phase stability, structural properties and vibrational modes. However, applying this approach to large systems, e.g., systems with thousands of atoms, remains a challenge even with contemporary computational platforms.

We will illustrate new algorithms to extend computations to suh systems. Our approach centers on solving the Kohn-Sham equation by a nonlinear form of subspace iteration. This approach results in a significant speedup, often by more than an order of magnitude with no loss of accuracy. We present numerical results for nanoscale systems with tens of thousands of atoms and propose new methods to extend our work to even larger systems.

Invited: Discontinuous projection method for large, accurate electronic structure calculations

John Pask
LLNL, Livermore, USA

For decades, the planewave (PW) pseudopotential method has been the method of choice for large, accurate Kohn-Sham calculations of condensed matter systems, in ab initio molecular dynamics simulations in particular. However, due to its reliance on a Fourier basis, the method has proven notoriously difficult to parallelize at scale, thus limiting the length and time scales accessible. In this talk, we discuss new developments aimed at increasing the scales accessible substantially, while retaining the fundamental simplicity, systematic convergence, and generality instrumental to the PW method's success in practice. The key idea is to release the constraint of continuity in the basis set, and with the freedom so obtained, employ a basis of local Kohn-Sham eigenfunctions to solve the global Kohn-Sham problem. In so doing, the basis obtained is highly efficient, requiring just a few tens of basis functions per atom to attain chemical accuracy, while simultaneously strictly local, orthonormal, and systematically improvable. We show how this basis can be employed to accelerate current state-of-the-art real-space methods substantially by reducing the dimension of the real-space Hamiltonian by up to three orders of magnitude. Results for metallic and insulating systems of up to 27,000 atoms using up to 38,000 processors demonstrate the scalability of the methodology in a discontinuous Galerkin formulation. Proceeding via reduction of the real-space Hamiltonian instead promises to reach larger scales still.

Quantum Many-body 1

Conference Center, Ballroom C

Invited: Langevin QMC algorithm for strongly interacting electron-phonon systems: The phase diagram of two-dimensional model with long range interactions

G George Batrouni[1,2,3], Richard Scalettar[4]

[1]Université Côte d'Azur, INPHYNI, CNRS, Nice, France. [2]Beijing Computational Science Research Center, Beijing, China. [3]MajuLab, CNRS-UNS-NUS-NTU International Joint Research Unit UMI 3654, Singapore, Singapore. [4]Department of Physics, University of California, Davis, USA

We present a quantum Monte Carlo algorithm for electron-phonon systems based on the Langevin equation. We discuss systematic errors due to discretization of Langevin time, autocorrelation, and the discretization of imaginary time (Trotter-Suzuki). We also discuss and implement Fourier acceleration to speed up convergence. We show that the execution time scales almost linearly with system size and demonstrate that, in the case of the Holstein model, the results are in excellent agreement with determinant QMC (which has cubic dependence on system size). We then use this algorithm to calculate, for the first time, the phase diagram of the strongly interacting electron-phonon system in two dimensions with long range interactions. We find a charge density (CDW) phase and a region of phase separation. We also examine the finite temperature phase transition.

Invited: Near-Term Quantum Algorithms for Quantum Many-Body Systems

Mark B Ritter[1], Kristan Temme[1], Abhinav Kandala[1], Antonio Mezzacapo[1], Marco Pistoia[2], Richard Chen[1], Jay Gambetta[1]

[1]IBM T.J. Watson Reearch Center, Yorktown Heights, NY, USA. [2]IBM T.J. Watson Reearch Center, Yorktown Heights, NY, Qatar

There has been a good deal of work on algorithms to simulate quantum many-body systems with fault-tolerant quantum computers- those with full error correction. Fault-tolerant quantum computers of scale requisite to achieve computational advantage for these problems are likely over a decade away. Moreover, devices that we can build in the near term, called Noisy Intermediate Scale Quantum computers (NISQ), have too much noise to implement the long circuits required by these algorithms. We review heuristic, short-depth quantum algorithms more suited to NISQ computers; specifically, their scaling properties when applied to electronic and nuclear structure calculations, including Hamiltonian complexity with particle number, ansatz state preparation, convergence, and noise. We will present examples of actual quantum structure calculations with NISQ computers, as well as a newly-demonstrated error mitigation technique that significantly improves accuracy. We end with an outlook for "advantage" – when NISQ systems might excel conventional HPC approaches for comparable problems.

Monday, Parallel Sessions 2, 04:00PM-06:00PM

Machine Learning 2

Conference Center, Ballroom A

Tight Binding Molecular Dynamics with Electron Open Boundaries

Andrew Horsfield[1], Mario Zauchner[1], Tchavdar Todorov[2]
[1]Imperial College London, London, United Kingdom. [2]Queen's University Belfast, Belfast, United Kingdom

Non-equilibrium chemical reactions of metals in an aqueous environment are ubiquitous (e.g. corrosion, and batteries), but very challenging to simulate at the atomic scale. The difficulties are three fold: to describe the system, many hundreds of non-equivalent atoms are required; the system is at finite temperature with many atoms being mobile; chemical reactions are occurring with electrons entering and leaving the simulation cell. From this we can see that the essential ingredients of any successful simulation are: a reliable description of bonding that permits transfer of electrons; an efficient description of bonding suitable for molecular dynamics; a very efficient scheme for electron open boundaries. For the description of bonding we use Tight Binding. Here we will introduce the Hairy Probe method of open boundaries [1], including its simplified form suitable for electrochemical simulations [2].

[1] "Efficient simulations with electronic open boundaries", A.P. Horsfield, M. Boleininger, R. D'Agosta, V. Iyer, A. Thong, T. N. Todorov, and C. White, Phys. Rev. B 94 075118 (2016)

[2] "Efficient electron open boundaries for simulating electrochemical cells", Zauchner, M. G., Horsfield, A. P., and Todorov, T. N., Physical Review B, 97 045116 (2018)

Comparison and Validation of Recent Exchange-Correlation Functionals for First-Principles Simulations of Water

Michael LaCount, Francois Gygi
UC Davis, Davis, USA

The validation of density functionals in first-principles simulations requires a detailed statistical analysis in order to identify significant differences between functionals. We present results of first-principles molecular dynamics simulations of liquid water obtained with the recently proposed SCAN meta-GGA density functional[1]. Results are compared with those obtained with the PBE GGA density functional[2]. Estimates of the variance of pair correlation functions, number of hydrogen bonds and angular correlations are derived in order to determine the duration of simulations needed for statistically significant comparisons.

[1] J. Sun, A. Ruzsinszky, J. P. Perdew, Phys. Rev. Lett. 115, 036402 (2015).

[2] W. Dawson and F. Gygi, J. Chem. Phys. 148, 124501 (2018).

[3] http://quantum-simulation.org

[4] http://qboxcode.org

Supported by the Midwest Integrated Center for Computational Materials (MICCoM), as part of the Computational Materials Sciences Program funded by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences.

Learning materials properties from orbital interactions

Tien-Lam Pham[1,2,3], Hiori Kino[2,4], Takashi Miyake[2,3,5], Hieu-Chi Dam[6,2,4]
[1]Japan Advanced Institute of Science ant Technology, Nomi-Ishikawa, Japan. [2]CMI2, National Institute for Materials Science, Tsukuba-Ibaraki, Japan. [3]ESICMM, National Institute for Materials Science, Tsukuba-Ibaraki, Japan. [4]JST, PRESTO, Kawaguchi-Saitama, Japan. [5]CD-FMat, AIST, Tsukuba-Ibaraki, Japan. [6]Japan Advanced Institute of Science and Technology, Nomi-Ishikawa, Japan

We propose a novel descriptor named Orbital Field Matrix (OFM) for representing material structures in datasets of multi-element materials. The descriptor is based on the information regarding atomic valence shell electrons and their coordination. We show that these descriptors are highly applicable in predicting the physical properties of materials, including solids and molecules. Further, valuable insights on the materials data set can be obtained by mapping from descriptor space into a low embedded dimensional space. For crystalline solid systems based on transition metal/lanthanide metal alloys, we focus on the local magnetic moment and formation energies. And for molecular systems, we investigate the atomization energy of molecular systems. These quantities of the materials are calculated by using density functional theory. We demonstrate that these quantities can be accurately reproduced using simple nearest-neighbor regression and OFM, thus confirming the relevance of our descriptors. Using kernel ridge regressions and OFM, we could accurately reproduce the formation energy, the local magnetic moment, and the atomization energy calculated by density functional theory, with mean absolute errors of 0.03 (μB) and 0.10 (eV/atom), 6.29 (kcal/mol), respectively. We show that meaningful low dimensional representations can be extracted from the original descriptor using dimensionality reduction techniques. Intuitive prehension on the materials space, qualitative evaluation on the similarities in local structures or crystalline materials, and inference in the designing of new materials by element substitution can be performed effectively based on these low-dimensional representations.

Materials 2

Conference Center, Ballroom B

Energetics of intrinsic point defects in aluminium via orbital-free density functional theory

Ruizhi Qiu
Institute of Materials, China Academy of Engineering Physics, JIANGYOU, China

The formation and migration energies for various point defects, including vacancies and self-interstitials, in aluminium are systematically reinvestigated using the supercell approximation in the framework of orbital-free density functional theory. In particular, the finite-size effects and the accuracy of various kinetic energy density functionals are examined. It is demonstrated that as the supercell size $N_s$increases, the finite-size errors asymptotically decrease as $O(1/N_s^3)$. Notably, the formation energies of self-interstitials converge much more slowly than that of vacancies. With carefully chosen kinetic energy density functionals, the calculated results agree quite well with the available experimental data and those obtained through Kohn–Sham density functional theory,which has an exact kinetic term.

Multiscale simulation of three-dimensional thin-film lubrication systems

Zuo-Bing Wu
LNM, Institute of Mechanics, Chinese Academy of Sciences, Beijing, China. School of Engineering Science, University of Chinese Academy of Sciences, Beijing, China

A multiscale simulation method that melds an atomistic description of the interfacial region with a coarse-grained description of the far region of the solid substrate is presented and applied to a three-dimensional model contact consisting of solid substrate and wall separated by a monolayer fluid film. Local and nonlocal elements are placed in the coarse-grained substrate, respectively. The hybrid method yields results in excellent agreement with the fully atomistic results. The importance of a proper accounting for the elastic response of the substrate, which is reliably and efficiently accomplished through coarse-graining of the far region, is demonstrated. Moreover, shearing transitions of multi-layer molecularly thin-film lubrication systems in variations of the film-substrate coupling strength and the load are studied by using the multiscale method. This research is supported by the National Natural Science Foundation of China through the Grants No. 11172310 and No. 11472284.

Development of a Multi-center Density Functional Tight Binding Model for Plutonium Surface Hydriding

Nir Goldman[1,2], Balint Aradi[3], Rebecca Lindsey[1], Laurence Fried[1]
[1]Lawrence Livermore National Laboratory, Livermore, USA. [2]University of California, Davis, USA. [3]University of Bremen, Bremen, Germany

We detail the creation of a multi-center density functional tight binding (DFTB) model for hydrogen on δ-plutonium, using a framework of new Slater-Koster interaction parameters and a repulsive energy based on the Chebyshev Interaction Model for Efficient Simulation (ChIMES), where two and three-center atomic interactions are represented by linear combinations of Chebyshev polynomials. We find that our DFTB/ChIMES model yields a total electron density of states for bulk δ-Pu that compares well to that from Density Functional Theory, as well as to a grid of energy calculations representing approximate

H_2 dissociation paths on the δ-Pu (100) surface. We then perform molecular dynamics simulations and minimum energy pathway calculations to determine the energetics of surface dissociation and subsurface diffusion on the (100) and (111) surfaces. Our approach allows for the efficient creation of multi-center repulsive energies with a relatively small investment in initial DFT calculations. Our efforts are particularly pertinent to studies that rely on quantum calculations for interpretation and validation, such as experimental determination of chemical reactivity both on surfaces and in condensed phases.

Exotic van der Waals interactions in graphene: from ultra-long ranged attraction to ultra-strong screening

Alberto Ambrosetti, Pier Luigi Silvestrelli
University of Padua, Padua, Italy

The Lifshitz-Zaremba-Kohn (LZK) theory is commonly regarded as the correct large-distance limit for the van der Waals (vdW) interactions between adsorbates and extended substrates. However, recent experiments are challenging the universality of the LZK theory over a broad spectrum of nanoscale materials. By overcoming the conventional local permittivity approximation, here we demonstrate that physical adsorption on graphene and other low-dimensional materials can exhibit highly non-trivial features. Substrate-adsorbate vdW interactions can be extremely long-ranged and externally tunable. Moreover, graphene can effectively screen weakly interacting supporting substrates, emerging as an effective tool for the experimental modulation of adsorption processes.

Spectrum Shifts in H_3S due to Strong Coupling to Phonons

Soham Ghosh, Warren Pickett
Department of Physics, University of California Davis, Davis, USA

A favorable combination of strong electron-phonon coupling, high phonon frequency and high density of states (DOS) near the Fermi energy exists in bcc H_3S[1] which was discovered to have a superconducting critical temperature T_c = 200 K at $\tilde{1}$60 – 200 GPa. We have employed first principles methods to analyze effects of the two van Hove singularities (vHs) which create a narrow peak of the electron DOS in this material. We use the EPW[2, 3] code to compute electron and phonon states on a dense Brillouin zone (BZ) integration mesh to obtain converged results. We demonstrate that electron spectral density shifts due to virtual phonon excitations leads to strong modification of the quasiparticle density of states. Unlike the commonly held expectation of smearing of peaks, we find that the DOS peak at the Fermi level is narrowed. These results illustrate that a DOS peak at the Fermi level requires treatment beyond conventional Eliashberg theory, to obtain quantitative results for superconducting and infrared properties of H_3S.

References:

[1] A. P. Drozdov, M. I. Eremets, I. A. Troyan, V. Ksenofontov, and S. I. Shylin. *Nature* volume 525, pages 73–76, September 2015.

[2] Feliciano Giustino, Marvin L. Cohen, and Steven G. Louie. Phys. Rev. B, 76:165108, Oct 2007.

[3] S. Ponc, E.R. Margine, C. Verdi, and F. Giustino. Computer Physics Communications, 209:116 – 133, 2016.

Electronic structure of square planar nickelates revisited: relationship to cuprates

Antia S. Botana[1], Junjie Zhang[1], John Freeland[1], Victor Pardo[2], Hong Zheng[1], Daniel Phelan[1], John Mitchell[1], Michael Norman[1]
[1]Argonne National Lab, Lemont, USA. [2]Universidade de Santiago de Compostela, Santiago de Compostela, Spain

The physics behind high-temperature superconducting cuprates remains a defining problem in Condensed Matter Physics. One way of addressing this problem has been to search for alternative transition metal oxides with comparable structures and *3d* electron count, proxies for cuprate physics. Based on electronic structure calculations, we propose low-valence layered nickelates ($R_4Ni_3O_8$, R=La, and Pr) as one of the closest analogs to cuprates. In particular, $Pr_4Ni_3O_8$ is metallic, exhibits a low-spin configuration of Ni, and significant orbital polarization with pronounced Ni-$d_{x^2-y^2}$ character near the Fermi energy, as well as a high degree of *d-p* hybridization. This compound offers entree to the region of *3d* electron count of hole-doped superconducting cuprates that can be achieved by electron doping.

Probing the Origin of High Temperature Superconductivity in H-rich Compounds

Yundi Quan, Warren Pickett
University of California Davis, Davis, USA

The discovery of record high temperature superconducting H3S in the 160-200 GPa regime, following remarkably a computational prediction, has reinvigorated interest in improving numerical methods for understanding conventional superconductivity based on conventional phonon pairing and strong coupling Eliashberg theory. Despite tremendous increase in computing power over the past few decades, achieving convergence of intermediate results and the electron-phonon coupling constant with respect to k- and q-mesh in the Brillouin zone using first-principles linear response calculations is rarely achieved. Due to Giustino and coworkers, Wannier function based methods have been formulated and implemented in the Electron-Phonon Wannier (EPW) code. This formulation provides very substantial speedup over previous methods. Using the EPW code, we systematically survey the class of predicted high temperature superconducting hydrides XH6, X= Mg, Ca. One emphasis has been on the numerical convergence of intermediate and final quantities, and providing analysis that leads to understanding of large variations in the predicted Tc whose origins are not readily seen. While pressure tends to increase interatomic force constants and thus higher phonon frequencies, it also suppresses electron-phonon coupling strength, which is inversely proportional to the square of the mean phonon frequency. The net result for Tc versus pressure depends on several apsects, which can be obtained with clear analysis.

Large anomalous Nernst and spin Nernst effects in noncollinear antiferromagnets Mn3X (X=Sn,Ge,Ga)

Guang-Yu Guo, Tzu-Cheng Wang
Department of Physics, National Taiwan University, Taipei City, Taiwan

Noncollinear antiferromagnets have recently been attracting considerable interest partly due to recent surprising discoveries of the anomalous Hall effect (AHE) in them and partly because they have promising applications in antiferromagnetic spintronics. Here we study the anomalous Nernst effect (ANE), a

phenomenon having the same origin as the AHE, and also the spin Nernst effect (SNE) as well as AHE and the spin Hall effect (SHE) in noncollinear antiferromagnetic Mn3X (X = Sn, Ge, Ga) within the Berry phase formalism based on ab initio relativistic band structure calculations. For comparison, we also calculate the anomalous Nernst conductivity (ANC) and anomalous Hall conductivity (AHC) of ferromagnetic iron as well as the spin Nernst conductivity (SNC) of platinum metal. Remarkably, the calculated ANC at room temperature (300 K) for all three alloys is huge, being 10–40 times larger than that of iron. Moreover, the calculated SNC for Mn3Sn and Mn3Ga is also larger, being about five times larger than that of platinum. This suggests that these antiferromagnets would be useful materials for thermoelectronic devices and spin caloritronic devices. The calculated ANC of Mn3Sn and iron are in reasonably good agreement with the very recent experiments. The calculated SNC of platinum also agrees with the very recent experiments in both sign and magnitude. The calculated thermoelectric and thermomagnetic properties are analyzed in terms of the band structures as well as the energy-dependent AHC, ANC, SNC, and spin Hall conductivity via the Mott relations.

Quantum Many-body 2

Conference Center, Ballroom C

Excitonic Coupled-cluster Theory for Large-scale Electronic Structure Calculations

Anthony D. Dutoi, Yuhong Liu
University of the Pacific, Stockton, CA, USA

One shortcoming of presently available fragment-based electronic structure methods is that electron correlation (if included) is modeled at the level of individual electrons, effectively recomputing local many-body fluctuations for each separate inter-fragment interaction. However, without approximation, the *ab initio* Hamiltonian may be rewritten in terms of subsystem fluctuations between locally correlated states (the exciton basis). Traditional electronic structure methods can then be applied directly to these renormalized coordinates.

Using this foundation, we have developed a working excitonic coupled-cluster (X-CC) code. We have acquired promising results on test systems of chains of Be atoms. The Be dimer is already a notoriously difficult multiconfigurational, semicovalent problem, for which charge transfer terms are essential. In a toy 6-31G basis, our method can handle 100 Be atoms (200 active electrons) in about 11 minutes, achieving a total dissociation energy comparable to conventional coupled-cluster theory with single and double orbital substitutions (CCSD). A calculation of this size presents challenges for production-level conventional CCSD codes, and further optimizations of the X-CC code are still pending.

The X-CC approach offers a robust avenue to embed difficult electronic structure problems in large, complex environments. An extension to excited states (therefore electron dynamics) is also straightforward.

Finite-Temperature Lanczos Method and its Application on Spin Frustrated Systems

Liangjian Zou[1,2], Yamin Quan[1], **H.-Q. Lin**[3]
[1]Institute of Solid State Physics, Chinese Academy of Sciences, Hefei, China. [2]University of Science and Technology of China, Hefei, China. [3]Beijing Computational Sciences Research Center, Beijing, China

Searching for exotic quantum states in magnetic frustrated systems remains a huge challenging task due to the highly entangled nature of spin frustrated systems. Among which the possibility of spin liquid phase remains a hot debated topic, especially in honeycomb lattice. Up to date most of literature focus on the zero-temperature groundstate properties of spin frustrated models; on the other hand, one may expect that the finite-temperature properties might display unusual characters of exotic spin quantum state. In this work we develop finite-temperature Lanczos algorithm based on finite-temperature and low-temperature Lanczos methods. In our program package, the reorthogonalization method is adopted to correct for the loss of orthogonality and the parallelization of our program is realized based on OPENMP parallel algorithm. Our algorithm could be used to calculate finite-temperature properties of finite-size quantum spin systems, and is applied on the J1-J2 Heisenberg and the Kitaev models on finite-size honeycomb lattice. For the J1-J2 Heisenberg models, we confirm that a quantum critical point exists at J2/J1=0.31 from zero to finite temperatures; for the Kitaev models, we demonstrate unusual specific heat, magnetic susceptibility and Wilson ratio in finite temperatures and finite magnetic field.

Game of Mixed Entangled States for Social Advantage

Aritra Das[1], Pratyusha Chowdhury[2]
[1]Dept. of Physics, Indian Institute of Technology Kanpur, Kalyanpur, UP, India. [2]Dept. of Physics, St. Xavier's College, Kolkata, India

It has been extensively shown in past literature that Bayesian Game Theory and Quantum Non-locality have strong ties between them. Pure Entangled States have been used, in both common and conflict interest games, to gain advantageous payoffs, both at the individual and social level. In this paper we construct a game for a Mixed Entangled State such that this state gives higher payoffs than classically possible, both at the individual level and the social level. Also, we use the I-3322 inequality so that states that aren't helpful as advice for Bell-CHSH inequality can also be used. Finally, the measurement setting we use is a Restricted Social Welfare Strategy (given this particular state).

Random-Singlet Phase in Disordered Two-Dimensional Quantum Magnets

Lu Liu[1], Hui Shao[2], Yu-Cheng Lin[3], Wenan Guo[1], **Anders Sandvik**[4]
[1]Beijing Normal University, Beijing, China. [2]Beijing Computational Science Research Center, Beijing, China. [3]National Chengchi University, Taipei, Taiwan. [4]Boston University, Boston, USA

We study effects of disorder in a 2D square-lattice S=1/2 quantum spin system, the J-Q model with a 6-spin interaction Q supplementing the Heisenberg exchange J. In the absence of disorder the system hosts antiferromagnetic and columnar valence-bond-solid ground states. The VBS breaks Z_4 symmetry, and in the presence of arbitrarily weak disorder it forms domains. Using QMC simulations, we demonstrate two kinds of such disordered VBS states. Upon dilution, a removed site leaves a localized spin in the opposite sublattice. These spins form AFM order. For random interactions, we find a different state, with no order but algebraically decaying mean correlations. We identify localized spinons at the nexus of domain walls between different VBS patterns. These spinons form correlated groups with the same number of spinons and antispinons. Within such a group, there is a strong tendency to singlet formation, because of spinon-spinon interactions mediated by the domain walls. Thus, no long-range AFM order forms. We propose that this state is a 2D analog of the well-known 1D random singlet (RS) state. The RS state discovered here in a system without geometric frustration should correspond to the same fixed point as the RS state recently proposed for frustrated systems, and the ability to study it without Monte Carlo sign problems opens up opportunities for further detailed characterization of its static and dynamic properties. We discuss possible experimental observations of this phase in triangular- and square-lattice quantum magnets.

Universality Class and Dangerously Irrelevant Field at Classical and Quantum Phase Transitions

Hui Shao[1,2], Pranay Patil[3], Wenan Guo[2], Anders Sandvik[3]
[1]Beijing Computational Science Research Center, Beijing, China. [2]Beijing Normal University, Beijing, China. [3]Boston University, Boston, USA

Previous studies have shown that the phase transitions between the paramagnet phase and the Z_q symmetry breaking phase in the classical 3D q-state clock models belong to the 3D XY universality class for q>4, which means that the Z_q field is irrelevant at the critical point. However, for any T<Tc, it is always relevant as the symmetry is broken discretely. This is "dangerous" because it leads to a larger

length scale ξ' than the normal correlation length ξ, which governs the crossover behavior from U(1) to Z(q) symmetry breaking. There are several proposals of the relationship between the associated critical exponents ν and ν', all of which seem to be roughly consistent with numerical calculations. By using proper physical observables related to the various fixed points, we have managed to construct quantitive Monte Carlo based RG flows, where the crossover behavior is clearly observed and quantified. Furthermore, due to the analogy between this classical phenomenon and deconfined quantum criticality (a continuous transition between an antiferromagnet and a 4-fold degenerate dimerized phase in two dimensions), we can also apply the same ideas in the quantum case and obtain additional insights into deconfined quantum criticality.

Numerical implementation for evaluating vertex corrections to electrical conductivity in multi-band electron systems

Giacomo Resta, Sergey Savrasov
University of California Davis, Davis, California, USA

Linear response electrical conductivity is often evaluated under the Kubo-Greenwood formalism by including only the Drude conductivity diagram and ignoring interaction-dressed vertex corrections. However, this approach is only valid for systems with isotropic scattering such as in the case where a single-band approximation is appropriate and the irreducible vertex function is k-independent (ex. short range impurities). In multi-band systems or in cases where the irreducible vertex function has a k-dependence (ex. long range impurities), vertex diagrams can provide a significant correction to the Drude conductivity. In particular, the multi-band nature of the Fermi surface plays an important role in the transport phenomena of many topological materials of recent interest such as topological insulators and semi-metals. In this talk, I will be discussing our recent numerical implementation for evaluating the leading-order vertex correction to the electrical conductivity of multi-band systems based on a numerically efficient projection scheme. Finally, I will demonstrate the important role of the vertex correction in the magnetotransport properties of Dirac semimetals in the presence of long range impurity potentials where the combination of k-dependent scattering and the multi-band nature of the wave-functions leads to the chiral anomaly.

This work was supported by the US National Science Foundation Grant DMR-1411336 (S.Y.S).

World-line Quantum Monte Carlo Simulation of the Extended Hubbard-Holstein Model with Long-range Electron-Phonon Interaction

Bo Xiao[1], Frederic Hebert[2], George Batrouni[2], Richard Scalettar[1]
[1]Department of Physics, University of California, Davis, USA. [2]Université Côte d'Azur, INPHYNI, CNRS, Nice, France

Quantum Monte Carlo (QMC) method is a powerful tool to understand the physics of strongly correlated interacting quantum system. Persistent questions concerning the role of phonons in strongly correlated materials like manganites, cuprates, iron pnictides , and organic superconductors keep the study of electron-phonon Hamiltonians at the forefront of research. We use world-line quantum Monte Carlo (WLQMC) to explore the ground state and finite temperature properties of one-dimensional many-body systems based on the extended Hubbard-Holstein Hamiltonian. This method is based on a direct-space, imaginary-time representation of the fermion and boson fields, which allows us to describe the regimes with dominant charge-density-wave, spin-density-wave, phase-separated ground states, superconductivity and metallic behavior. We apply this method to explore the essential influence of

electron-phonon interaction which ranges from the Holstein to the Fröhlich regime. We used WLQMC simulations to study many-electron systems with long-range interaction and presented phase diagrams in different regions of the phase space.

Study of the influence of structural defects on the optoelectronic properties of two dimensional transition metal dichalcogenides.

Himani Mishra, Sitangshu Bhattacharya
Indian Institute of Information Techonology, Allahabad, India

Single layer transition metal dichalcogenides (TMDCs), direct band gap semiconductors have attracted a lot of research and study due to their excellent electro-optical integrity. Optical absorption within these monolayers is extremely influenced by the presence of structural defects. At reduced dimensions the interaction between these defect created trap centres and charge carriers becomes more prominent leading to the formation of bound excitons. Here we demonstrate the absorption spectra of a single layer MoS_2 and WSe_2 through many body perturbation theory in the presence of structural defects prominent in these monolayers. We use a fully relativistic approach within the non-self-consistence GW approximation containing the nonlinear core correction with full spinor wave functions. The absorption spectra calculation is achieved through the full Bathe-Salpeter equation to include the excitonic excitations. Our computations exhibit a Gaussian absorption spectra observed with double excitonic peaks A and B, unlike the step function profile without the incorporation of excited states. This double peak corresponds to valence band splitting at the K point of the brillouin zone and is a result of spin orbit splitting of the valence band maximum. The absorption edge demonstrates a red shift when investigated in the presence of defects which can be attributed to inter excitionic interactions and the reduction in bandgap in the presence of defects. A reduction in the value of absorption coefficient is observed as a result of localization of excitons in the traps. Our outcomes clarify the defect and exciton material science, offering another course towards fitting its physical properties by defect engineering.

Tuesday, Parallel Sessions 1, 02:00PM-03:30PM

Astrophysics 1

Conference Center, Ballroom A

Invited: The Convergence of HPC and Big Data in Cosmology

Peter Nugent
LBNL, Berkeley, USA

In recent years astrophysics has undergone a renaissance, transforming from a data-starved to a data-driven science. A new generation of experiments — including Planck, BOSS, DES, DESI, Euclid, WFIRST and LSST — will gather massive data sets that will provide more than an order of magnitude improvement in our understanding of cosmology and the evolution of the universe. Their analysis requires leading-edge high performance computing resources and novel techniques to handle the multiple PB's of data generated throughout these surveys. Furthermore, interpreting these observations is impossible without a modeling and simulation effort that will generate orders of magnitude more "simulation" data — used to directly understand and constrain systematic uncertainties in these experiments and to determine the covariance matrix of the data. As we enter this era of precision cosmology a thorough propagation of errors on measurements in both the experiments and simulations becomes essential. This is especially true in modern cosmological models where many parameters and measurements are partially degenerate, and such degeneracies can lead to important shifts in the cosmological parameters one is trying to measure.

Invited: Simulations of Core-Collapse Supernova Explosions

Joshua Dolence
Los Alamos National Laboratory, Los Alamos, USA

Core-collapse supernovae are the explosive deaths of massive stars. They seed the Universe with many of the elements essential for life, are the birth places of neutron stars and black holes, and may serve as a unique probe of physics under exotic conditions. Despite decades of effort, the mechanism that transforms the collapse of a massive star into one of Nature's most remarkable events is still incompletely understood, but large-scale multi-physics simulations provide for critical insights into these complex phenomena. State-of-the-art supernova modeling involves all four-fundamental forces and an enormous dynamic range of length- and time-scales. The dynamics are fundamentally three-dimensional, highly nonlinear, chaotic, and span a huge range of physical regimes. These features come together to form an exceptionally challenging computational problem that requires sophisticated codes that scale on the largest available machines. In this talk, I will discuss the status of core-collapse supernova modeling and the tools of the trade, with an emphasis on the results, methods, and algorithms of the Fornax code.

Materials 3

Conference Center, Ballroom B

Invited: Computational Discovery of New Materials Under Pressure

Eva Zurek
University at Buffalo, SUNY, Buffalo, USA

The pressure variable opens the door towards the synthesis of materials with unique properties, e.g. superconductivity, hydrogen storage media, high-energy density and superhard materials. Under pressure elements that would not normally combine may form stable compounds or they may mix in novel proportions. As a result, we cannot use our chemical intuition developed at 1 atm to predict phases that become stable when compressed. To enable our search for novel hydride phases that can be synthesized under pressure we have developed *XtalOpt*, an open-source evolutionary algorithm for crystal structure prediction. *XtalOpt* has been employed to find the most stable structures of hydrides with unique stoichiometries. Some of these are superconducting at high temperatures. Herein, we describe our predictions of the binary hydrides of scandium, phosphorus, calcium and iron. The electronic structure and bonding of the predicted phases is analysed by detailed first-principles calculations.

Invited: Cumulant Green's function approach for excited states, response functions, and thermodynamics

John J. Rehr
University of Washington, Seattle, USA

A quantitative treatment of electronic excitations and response functions in condensed matter has long been challenging. Physically, these properties depend on many-body correlation effects ignored in independent particle approximations. Quasi-particle (QP) approaches yield significant improvements, as in GW and GW/Bethe-Salpeter equation methods [1], but ignore inelastic losses due to multi-electron excitations. Recently there has been considerable interest in the cumulant Green's function approach [2,3] which addresses this behavior. In contrast to GW, this approach explains multiple-plasmon satellites and charge-transfer excitations observed in XPS, as well as the many-body amplitude factors S_0^2 in EXAFS. We also discuss the finite temperature (FT) extension [4], with a cumulant based on the Matsubara Green's function. The method yields FT exchange-correlation potentials and energies for FT-DFT (density functional theory) and FT-TDDFT, in good agreement with quantum-Monte Carlo calculations. The method is illustrated with a number of applications including thermodynamic properties of the homogeneous electron gas over a wide range of densities and temperatures from cool to the warm dense matter (WDM) regime [4].

Acknowledgment: Supported by DOE BES TCMP Grant DE-FG02-97ER45623.

[1] K. Gilmore et al., Comput. Phys. Comm. **197**, 109 (2015).

[2] L. Hedin, J. Phys.: Condens. Matter **11,** R489 (1999).

[3] J. Sky Zhou et al., J. Chem. Phys. **143**, 194109 (2015).

[4] J. J. Kas and J. J. Rehr, Phys. Rev. Lett. **119**, 176403 (2017).

Software 1

Conference Center, Ballroom C

Invited: Quantum algorithms for simulating quantum field theories

Stephen Jordan[1,2], John Preskill[3], Keith Lee[4], Ali Moosavian[5], Hari Krovi[6]
[1]Microsoft Research, Redmond, USA. [2]University of Maryland, College Park, USA. [3]Caltech, Pasadena, USA. [4]U. Toronto, Toronto, Canada. [5]U. Maryland, College Park, USA. [6]Raytheon/BBN, Cambridge, USA

Quantum field theory lies at the heart of both condensed-matter and high energy physics. In some parameter regimes, extracting quantitiative predictions from quantum field theories, particularly regarding dynamical quantities such as scattering probabilities, appears to be intractable using conventional techniques. Here I will discuss new advances in quantum algorithms for simulating quantum field theories which achieve exponential speedup over known classical algorithms and polynomial speedup over prior quantum algorithms. Prior knowledge of quantum field theory will not be assumed. This is joint work with Keith Lee, John Preskill, Hari Krovi, and Ali Moosavian.

Invited: Efficient Methodologies for Optimization and Control in Fluid Mechanics

Nicolas Gauger
TU Kaiserslautern, Kaiserslautern, Germany

At the beginning of the talk we discuss how to set up robust adjoint solvers for optimization and control in fluid mechanics in an automated fashion by the advanced use of algorithmic differentiation (AD). Then we discuss how to extend the resulting fixed-point solvers into so-called one-shot methods, where one solves the optimality system consisting of the primal, the dual/ adjoint and the design equations simultaneously. This is discussed for steady state cases first and then extended to unsteady partial differential equations (PDEs). Integrating existing solvers for unsteady PDEs into a simultaneous optimization method is challenging due to the forward-in-time information propagation of classical time-stepping methods. We apply the simultaneous single-step one-shot optimization method to a reformulated unsteady constraint that allows for both forward- and backward-in-time information propagation. Especially in the presence of chaotic and turbulent flow, solving the initial value problem simultaneously with the optimization problem often scales poorly with the time domain length. The new formulation relaxes the initial condition and instead solves a least squares problem for the discrete partial differential equations. This enables efficient one-shot optimization that is independent of the time domain length, even in the presence of chaos.

Tuesday, Parallel Sessions 2, 04:00PM-06:00PM

Astrophysics 2

Conference Center, Ballroom A

Propagation of Dust-Ion Acoustic Solitary Waves in Dusty Plasma with Boltzmann Electron

Samiran Das
Central Institute of Technology Kokrajhar, Kokrajhar (Assam), India

In this multispecies plasma model, consisting of negative charged mobile dusts, non-thermal ions and Boltzmann electrons, dust-ion acoustic solitary waves are studied through reductive perturbative technique by deriving corresponding Korteweg-de Vries (KdV) equation. The number of dust charge contained in a dust particle and the initial dusts speeds (u_{d0}) and ions (u_{i0}) are observed to play very important role to form dust-ion acoustic compressive and rarefactive KdV solitons. Remarkably, some initial dust speed (u_{d0}) are found to be instrumental for both compressive and rarefactive KdV solitons in a short range of Z_d separating both kinds by some asymptotic lines. Also, the presence of low dust charges and lower ion streaming, compressive and rarefactive KdV solitons of either concave or convex characters are shown to reflect. For the higher value of u_{d0}, the amplitudes of the rarefactive KdV solitons characteristically changes from higher to lower values showing convex character for this plasma model. A rigorous theoretical investigation has been made to show how the number of dust charge contained in a dust particle (Z_d) drastically change the amplitudes of the compressive and rarefactive KdV solitons. Also, the existence of this plasma model in some astrophysical and space plasma systems, especially to planetary ring-systems and cometary tails etc. are briefly reported.

The Angular Fractal Dimension as a Measure of the Inhomogeneity in the Galaxy Clusters Distribution in the Redshift Range (Z=0-1)

Loay Khalifa[1], Jesus Pando[2]
[1]DePaul University, Chicago, USA. [2]DePaul University, Chicago, USA

The study of large-scale structure (LSS) of the universe armed with both all-sky surveys and numerical simulations has become an increasingly important tool to calculate different cosmological parameters. We developed a computational algorithm to calculate the angular fractal dimension D as a function of redshift using the Baryon Oscillation Spectroscopic Survey (BOSS) and Mock Galaxy Catalogs produced by the Sloan Digital Sky Survey (SDSS). We used the wavelet packet transform and the fractal based-point processes statistics as our main tools. Taking advantage of the self-similarity and localization properties of the wavelets, allows us to compute the fractal dimension of galaxies at narrow redshift bins. We found D to be in the range (1.5-1.7) and presented the evidence that galaxy clusters behave as fractal systems in the redshift range Z = 0.1 to Z = 1. We found also that the fractal dimension decreased as the redshift increased. We concluded that the galaxy clusters distribution is inhomogeneous in that redshift range. Finally, we concluded that the large-scale structure of the universe was dominated by voids in the past.

Higher-order Vlasov-Poisson Simulation for Large-Scale Simulation with Massive Neutrino

Satoshi Tanaka[1], Kohji Yoshikawa[1], Naoki Yoshida[2,3]
[1]University of Tsukuba, Tsukuba, Ibaraki, Japan. [2]University of Tokyo, Bunkyo, Tokyo, Japan. [3]Kavli Institute for the Physics and Mathematics of the Universe, Kashiwa, Chiba, Japan

We present a higher-order scheme for Vlasov simulations in six-dimensional phase-space for collisionless system. This scheme achieves spatially seventh order accuracy while ensuring the monotonicity and positivity of numerical solutions that the distribution function should satisfy. Such a higher-order scheme enables higher spatial resolution for a given number of mesh grids and, thus is essential in performing Vlasov simulations in six-dimensional phase-space because they consume huge amount of memory. Furthermore, we present a series of cosmological Vlasov-Poisson simulations of neutrino in the large-scale structure in the universe. Conventional N-body simulations are not very good at handle the collisionless damping (free-streaming) of massive neutrinos accurately because they are contaminated by the shot-noise due to Monte Carlo sampling of matter distribution. On the other hand, Vlasov-Poisson simulation is free from the shot-noise inherently and can handle the free-streaming effects accurately. Therefore, the results obtained with Vlasov-Poisson simulation of massive neutrinos presented in this talk can be considered to be the most reliable one ever investigated, and can be utilized to estimate the yet-to-be-determined physical properties of neutrinos (absolute mass and/or mass hierarchy) by being confronted with very large galaxy surveys planned in near future.

Simulating the Milky Way

Andrew Wetzel
UC Davis, Davis, USA

Within the cosmic web, galaxies like our own Milky Way form as gas flows along cosmic filaments into dark-matter halos, fueling the formation of stars, while the resultant feedback from stars drives strong outflows of gas. Understanding this nonlinear interplay between cosmic inflows and feedback-driven outflows is one of the most significant questions in astrophysics and cosmology, and it requires a new generation of supercomputer simulations that can achieve high dynamic range to resolve the scales of stars within a cosmological environment. I will describe how we are using massively parallelized cosmological zoom-in hydrodynamic simulations, run on the world's largest supercomputers, to model the physics of galaxy formation at unprecedented resolution. I will discuss new insight into the formation of our Milky Way galaxy, including the faint "dwarf" galaxies observed around it. These low-mass galaxies trace structure formation on the smallest cosmological scales and have presented the most significant challenges to the cold dark matter paradigm. I will describe how these new generations of simulations are allowing us to shed light on dark matter.

Data Reduction Using Lossy Compression for Cosmology and Astrophysics Workflows

Jesus Pulido[1,2], Zaija Lukic[3], Paul Thorman[4,1], Caixia Zheng[5], James Ahrens[2], Bernd Hamann[1]
[1]University of California Davis, Davis, USA. [2]Los Alamos National Laboratory, Los Alamos, USA. [3]Lawrence Berkeley National Laboratory, Berkeley, USA. [4]Haverford College, Haverford, USA. [5]Northeast Normal University, Changchun, China

In many of today's simulations, over trillions of cells are generated producing over terabytes of scien-

tific data per simulation step. Similarly, future observational datasets are projected to produce tens of Terabytes per day. Moving large amounts of data between simulation and observation nodes to disk introduces many I/O and storage bottlenecks. Limitations like these are constantly making compression techniques a viable choice for data reduction. While lossless techniques can compress large data with no loss of information, they do not produce a large-enough reduction compared to recent lossy methods. By using recent multi-resolution lossy compression techniques, large datasets can be reduced significantly while preserving coherent features and statistics required for post-analysis routines. Importantly, conducting lossy data compression introduces a net reduction in I/O transfer cost and enables the capability of storing more data at higher temporal frequency. In this work, we examine the results using multi-resolution lossy compression for data reduction on LSST simulation and AMReX/Nyx cosmology simulation data.

Measurement of the properties of neutron-star and black-hole binaries using PyCBC Inference

Soumi De
Syracuse University, Syracuse, USA

The LIGO and Virgo observatories have recently detected gravitational waves several binary black-hole and a binary neutron-star merger, opening a whole new field of gravitational wave and multi-messenger astronomy. We expect that in a few years from now, LIGO will detect a significant number of black-hole and neutron-star binary sources, allowing us to explore the masses, spins, distances, structure, and other properties of compact objects in the universe. Accurate measurement of the parameters of these real signals rather has become essential to extract information about the population, evolution, properties, and composition of their astrophysical compact-object sources. I will then present measurements of properties of some of the recent LIGO detections, using the PyCBC Inference software. PyCBC Inference is an open-source Python-based toolkit, that uses Bayesian inference methods for estimating the model parameters of compact-object mergers in gravitational-wave detector data. I will present the features and framework of the PyCBC Inference software. I will then highlight some of the recent results using this software, focusing mainly on the analysis of the gravitational-wave data of the recent binary neutron star detection - GW170817, incorporating information from nuclear matter studies and electromagnetic observations. The analysis is carried out with the crucial requirement that the two stars of GW170817 should obey a common equation of state. This is the first gravitational-wave parameter estimation analysis providing measurements of the neutron-star radius and tidal deformability, considering a physical constraint on the star's equation of state.

Materials 4

Conference Center, Ballroom B

Learning About Crystallography By Designing a Web Page

Michael Mehl
United States Naval Academy, Annapolis MD, USA

My first introduction to electronic structure calculations involved computing the total energy of MgO in the ”B1” (rock salt) and ”B2” (Cesium Chloride) structures, and later the ”A15” superconductors, which at the time were considered to be ”high-temperature.”

When I asked ”where do those labels come from?” I was told ”Strukturbericht,” which led me to the wonderful collection of a myriad of crystal structures published in prewar Germany.

Eventually my colleague and supervisor, Dimtrios Papaconstantopoulos, asked me if I would put together a series of web pages describing the Strukturbericht systems, including primitive lattice and atomic positions. This was the beginning of what we called the NRL Crystal Lattice Structure web page, which eventually grew to include nearly three hundred structures, with information not only on their periodic structure but also on the space group and Wyckoff positions. Of course that meant that I had to learn exactly what those things were, meaning I had to get further into the study of crystallography than I’d found in Kittel or Ashcroft and Mermin.

This talk will focus on the development of the NRL Crystal Lattice Structure page and its successor, the Library of Crystallographic Prototypes, part of the AFLOW consortium at Duke University (http://aflow.org/CrystalDatabase). I’ll talk about improvements to the site, how you can contribute to it, and how it can be used as an introduction to electronic structure calculations, even by undergraduates.

This work was funded by Duke University and the Kinnear Foundation.

Enabling accessible high-fidelity high-throughput computational design of electronic materials from first principles.

Protik Das, Mohammad Mohammadi, **Timur Bazhirov**
Exabyte Inc, San Francisco, USA

Recent advances in computational design from first principles enable high-throughput studies of large varieties of material compounds [1-3]. Two important limitations of previously used techniques are due to their limited ability to provide high fidelity in a controllable manner and limited accessibility to novel users. We report on the implementation of a novel approach, where high-fidelity first-principle simulation techniques, such as Density Functional Theory with Hybrid Screened Exchange (HSE) and GW approximation (G0W0) are standardized, made available in an easy-to-access way, and applied to a set of 100 semiconducting materials ranging from pure elements to III-V and II-VI compounds, ternary oxides and alloys. We calculated the electronic band gaps and band structures and compare the results with available experimental data. We find that for HSE and G0W0, the average relative error fits within 20-25%, whereas for conventional generalized gradient approximation-based approach it is within 50-60% range. For HSE we find the average calculation time to be approximately 30 hours on an up-to-date server centrally available from a public cloud provider, with the resulting average cost per material at approximately one hundred dollars. This work provides a cost-effective, accessible and repeatable practical recipe for performing high-fidelity first principle calculations of electronic materials in a high-throughput manner.

[1] Jain et. al., APL Materials, 1(1), 011002,

[2] Curtarolo et. al., Computational Materials Science, 58, 227-235,

[3] Pizzi et. al., Computational Materials Science, 111, 218-230.

Ab initio prediction of the structure of Extreme Nanowires Encapsulated within Cabon Nantoubes.

Jamie Wynn[1], Paulo Medeiros[1], Andrij Vasylenko[2], Jeremy Sloan[2], David Quigley[2], **Andrew Morris**[3]
[1]University of Cambridge, Cambridge, United Kingdom. [2]University of Warwick, Coventry, United Kingdom. [3]University of Birmingham, Birmigham, United Kingdom

The encapsulation of materials within single-walled carbon nanotubes (SWNT) affects their behaviour, structure and stability dramatically relative to bulk. In many cases, such extreme nanowires (ENWs) exhibit long-range ordered one-dimensional phases that do not, *or cannot,* exist in three-dimensions. Many are of technological interest, some with enhanced conductive[1] or thermoelectric properties[3]. Others, the so-called *nano phase-change materials*, have properties making them potential candidates for information storage technologies.

The prediction of encapsulated wires presents unique problems beyond bulk structure prediction. To predict a new phase within a SWNT, the simulated SWNT must be a commensurate length to the periodicity of the ENW, otherwise the lowest energy structures may have prohibitively large artificial strain. However, this periodicity is clearly only knowable *after* the candidate structure is predicted.

We have extended AIRSS for the prediction of quasi-1D crystals formed by materials encapsulated within nanotubes, allowing us to perform the first truly *ab initio* quantitative structure prediction calculations for ENWs. To illustrate the capabilities of the method, we present results for metal halides and chalcogens[3,4].

We map out the series of phase transitions occurring as the radius of the SWNT is varied and verify our predictions using TEM and ADF STEM.

[1] A. Vasylenko, et al. Phys. Rev. B (R) ***95*** *121408 (2017)*

[2] A. Vasylenko, et al. ACS Nano ASAP (2018), DOI:10.1021/acsnano.8b02261

[3] P. V. C. Medeiros,et al. ACS Nano ***11*** *6178-6185 (2017)*

[4]J. M. Wynn, et al. Phys. Rev. Mat. ***1*** *073001 (2017)*

Confinement-driven electronic and topological phases in corundum-derived oxide honeycomb superlattices

Okan Köksal, **Rossitza Pentcheva**
University of Duisburg-Essen, Duisburg, Germany

Using density functional theory calculations with a Hubbard *U* term, we investigate electronic, magnetic and possibly topologically non-trivial phases in X_2O_3 honeycomb layers confined in the corundum structure α-Al_2O_3 (0001). While the systems with = 3 cations show a trivial antiferromagnetic Mott insulating ground state, the ferromagnetic solutions of *X*= Ti, Mn, Co and Ni with constrained symmetry of the two sublattices exhibit a characteristic set of four bands associated with the single occupation of e_g' (Ti) and e_g (Mn, Co, Ni) states. Moreover, the Dirac point can be tuned to the Fermi level by strain and a significant anomalous Hall conductivity arises when spin-orbit coupling (SOC) is included. A particularly strong SOC effect is identified for *X* = Ti at a_{Al2O3}=4.81 Å accompanied by an unusually high orbital moment of -0.88 μ_B nearly quenching the spin moment of 1.01 μ_B. The emergence of this orbital magnetism makes the realization of Haldane's model of spinless fermions possible. The extension of this work to the 4*d* and 5*d* series led to the identification of cases of high orbital moment (Os) or candidates for Chern insulators (CI), i.e. *X* = Tc and Pt with C=-2 and -1, depending on the Coulomb repulsion strength. Parallels to the perovskite derived analogues are discussed. Support by the DFG, CRC/TRR80, G3 is gratefully acknowledged.

[1] O. Köksal, S. Baidya, and R. Pentcheva**,** Phys. Rev. B **97**, 035126 (2018).

[2] O. Köksal and R. Pentcheva, J. Phys. Chem. Solids, in press.

Computational study of functional properties in extreme nanowires

Andrij Vasylenko[1], Jamie Wynn[2], Paulo Medeiros[2], Jeremy Sloan[1], Andrew Morris[3], **David Quigley**[1]
[1]University of Warwick, Coventry, United Kingdom. [2]University of Cambridge, Cambridge, United Kingdom. [3]University of Birmingham, Birmingham, United Kingdom

Increasingly sophisticated synthesis techniques allow for experimental realisation of nanowires with cross sections of only a few (or even one) atomic diameter. One such synthesis involves crystallisation inside the confined environment of a single-walled carbon nanotube (SWCNT). The resulting "extreme nanowires" present an unprecedented opportunity to study functional properties at the smallest possible scale [1]. We will present results of two studies which combine *ab initio* calculations with solution of the Boltzmann transport equation to explore different of transport in these wires.

In the first, we demonstrate how the presence of a single atom diameter beryllium nanowire within an SWCNT provides additional thermalisation channels which alleviates the accumulation of "hot" phonons resulting in significantly enhanced electrical conductivity at high bias voltage [2].

In the second, we consider tin telluride extreme nanowires formed using the SWCNT as a template. TEM imagery combined with *ab initio* phonon calculations demonstrate formation of several nanowire structures which remain dynamically stable even without the templating SWCNT. One dimensional structures are expected to exhibit enhanced thermoelectric performance. We conduct non-equilibrium transport simulations based on an ab initio parameterised Boltzmann equation and demonstrate a factor of 6 improvement over the bulk material, reaching a figure of merit in excess of 3.0.

[1] C. E. Giusca *et al*, *Nano Lett.*, 2013, Vol. 13, pp4020–4027.

[2] A. Vasylenko *et alPhys. Rev. B* 2017, 95, 121408(R)/1-4 (2017).

[3] A. Vasylenko *et alACS Nano,* in press (2018).

Effects of chemical intercalation, strain and phase transition on heat transport in bulk and single-layer MoS_2: First-principles calculations

Shunda Chen[1], Aditya Sood[2], Bin Ouyang[3], Shiyun Xiong[4], Eric Pop[2], Kenneth Goodson[2], Davide Donadio[1]
[1]UC Davis, Davis, USA. [2]Stanford University, Stanford, USA. [3]UIUC, Urbana, USA. [4]Soochow University, Suzhou, China

The possibility of tuning the vibrational properties and the thermal conductivity of layered van der Waals materials either chemically or mechanically would open a way to significant advances in nanoscale heat management, which is of importance for potential applications in energy storage, nanoelectronics and optoelectronics. Here we investigate the effects of lithium intercalation, cross-plane strain and phase transition on heat transport in bulk and single-layer MoS_2, by first principles calculations. We find that both the in-plane and cross-plane thermal conductivity of bulk MoS_2 are extremely sensitive to both strain and electrochemical intercalation. Combining lithium intercalation and strain, the in-plane and cross-plane thermal conductivity can be tuned by one and two orders of magnitude, respectively. Furthermore, the thermal conductivity anisotropy of bulk MoS_2 can be modulated over two orders of magnitude. Upon phase transition from 1H phase to distorted 1T phase, the lattice thermal conductivity of single-layer MoS_2 is reduced by about one order of magnitude. The underlying mechanisms are uncovered by analyzing phonon dispersion relations, relaxation time and mean free paths. Our well converged, parameter-free calculations resolve discrepancies in the literature about the thermal conductivity of MoS_2, and our findings can be exploited to design novel phononic devices, as well as for thermal management in MoS_2-based electronics and optoelectronic systems.

Calculated Seebeck coefficient of transition-metal elements Calculated Seebeck coefficient of transition-metal elements

Sonju Ko[1], **Hisazumi Akai**[2]
[1]Graduate School of Engineering Science, Osaka University, Toyonaka, Japan. [2]Institute for Solid State Physics, The University of Tokyo, Kashiwa, Japan

Theoretical calculation of the Seebeck coefficient of transition metal elements has long been a challenging task. The reason is that, firstly, at T=0K, the conductivity of pure metal diverges. Second, the Fermi surfaces of transition metals composed of many different states where the simple constant relaxation time approximation does not work: this prevents us from cancelling out the relaxation time appearing in the numerator L_{12} and denominator L_{11} of the expression of the Seebeck coefficient that is proportional to L_{12}/L_{11}. To overcome the difficulty, we included the effects of electron-phono scattering in the calculation of the Seebeck coefficient. We exploited the Korringa–Kohn–Rostoker (KKR) Green's function method combined with the coherent potential approximation (CPA; KKR-CPA) and linear response theory. The approach combines three components: linear response theory in the framework of the KKR method; ab-initio phonon calculations; and an alloy analogy applied to the local static phonons using the KKR-CPA. The calculated Cu resistivity and Seebeck coefficients for various transition-metal elements at finite temperature show reasonably good overall agreement with experiment. The present approach provides a framework applicable to a wide range of materials, including pure metals, compounds, ordered and disordered alloys, opening up the possibilities of computational design of useful thermoelectric materials.

Edge-free graphene quantum dots on hexagonal boron nitride

Nils M. Freitag[1], Tobias Reisch[2], Peter Nemes-Incze[3], Joachim Burgdörfer[2], Markus Morgenstern[1], **Florian Libisch**[2]
[1]II. Institute of Physics B, JARA-FIT, RWTH Aachen University, Aachen, Germany. [2]Inst. f. Theoretical Physics, TU Wien, Vienna, Austria. [3]Centre for Energy Research, Institute of Technical Physics and Materials Science, Budapest, Hungary

Graphene offers two binary degrees: the electron spin and the valley. Efficient spin control has been demonstrated in many solid-state systems, whereas exploitation of the valley has only recently been started, albeit without control at the single-electron level. Here, we show that van der Waals stacking of graphene onto hexagonal boron nitride offers a natural platform for valley control. Aligning the two layers yields a superstructure with a periodicity of $\tilde{1}3$ nanometers. By combining electric and magnetic fields, we can smoothly confine electrons within the moire superstructure in both theory and experiment, and show that the smooth confinement allows for controlled manipulation of the valley degree of freedom [1].

Simulating this systems requires both high-level approaches vor describing the Van der Waals interaction between the layers, as well as large-scale tight binding and molecular dynamics techniques to describe the entire quantum dot. The resulting multi-scale model includes strain effects within the graphene membrane, the interaction with the substrate and the combined electric and magnetic fields. Our results compare well to direct measurements of the quantum dot states, yielding exquisite details of the graphene - boron nitride interaction.

[1]N. M. Freitag et al, Nature Nanotechnology **13**, 392-397 (2018)

Software 2

Conference Center, Ballroom C

Gaussian Tight Binding: like DFT, but much faster

Andrew Horsfield[1], Max Boleininger[2], Jana Smutna[1], Mark Wenman[1], Richard Fogarty[1]
[1]Imperial College London, London, United Kingdom. [2]CCFE, Abingdon, United Kingdom

There has been a recent resurgence in interest in the possibilities afforded by Tight Binding (TB): an inexpensive electronic structure method that is capable of delivering accuracy comparable to DFT but at a cost two to three orders of magnitude smaller. Here we present extended TB models that increase the domain of problems to which they can be applied: increased basis sets, inclusion of core electrons, and multipole expansions for the charge density [1] enable reliable simulations of the interaction of intense lasers with organic molecules [2]. For studies of metals in complex environments further evolution of the models is required: we will discuss the key ideas we are implementing for new models of Zr and Mg.

Two dimensional materials design by high-throughput calculations

Jun Zhou, Yuanping Feng, Lei Shen, Miguel Dias Costa
National University of Singapore, Singapore, Singapore

Two-dimensional (2D) materials, such as the prototype graphene, have attracted tremendous research interest for their unusual properties not found in their bulk forms and appealing applications in nano-scale electronics. A database for 2D materials could greatly accelerate the pace of development and deployment of new advanced atomically thin materials. Here, starting from the $\tilde{7}$0000 three-dimensional (3D) inorganic materials in Materials Project database, we screen around 2000 layered materials by a geometry-based algorithm. A top-down approach is applied by exfoliating these layered materials to monolayers with high-throughput calculations for their basic structural and electronic properties. In addition, a bottom-up approach by substitutions of the elements in the existing 2D materials from top-down approach with the ones in the same column of periodic table was adopted, which significantly expands the scale of the 2D material database. We use the 2D binary materials as an example and demonstrate that a comparable number of new stable 2D materials (energy-above-hull less than 100 meV/atom) could be generated by this approach.

Driving force dependence of the height of a faceted macrostep in non-equilibrium steady-state crystal growth

Noriko Akutsu
Osaka Electro-Communication University, Neyagawa, Osaka, Japan

Making good quality crystals of SiC is an urgent problem for the production of future power devices with low power consumption. Self-organized macrosteps are known to hinder making good quality of crystal of SiC [1]. We studied the largeness of the macrosteps theoretically based on a lattice model, the restricted solid-on-solid model with point-contact-type step-step attraction (p-RSOS model) [2]. We focus on the surface dynamics with the change of kink density or surface roughness, which has long been overlooked in studies of surface and volume diffusion. In our lattice model, a faceted macrostep exists on a vicinal surface stably even at equilibrium at low temperatures. The characteristics of the profile of the macrostep are classified by the connectivity of the surface free energy (or the surface tension) which was calculated by the density matrix renormalization group method [3]. Driving force dependence of the profile of vicinal surface with faceted macrosteps is analyzed by the Monte Carlo method [2]. Combining our results with the results calculated by Chernov and Nishinaga based on the volume diffusion will lead to a deep understanding of the formation of macrosteps.

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Simulated annealing, effective but inefficient? A case study for the 3D136 instance of the HP model of protein folding

Arnulf Möbius[1], Florian Günther[2]
[1]*Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden (IFW), Dresden, Germany.* [2]*Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Germany*

Because of its physical plausibility, the simulated annealing algorithm (SA) is very popular and is taught in most courses on computational physics. However, its efficiency seems to be rather weak. Thus, for the last decades, various new heuristic optimization approaches, e.g. thermal cycling, have been demonstrated to be clearly advantageous over SA. To keep such a comparison as fair as possible, we pushed SA to its limits for the 3D136 instance of the hydrophobic-polar lattice model of protein folding, a very difficult task. In doing so, we have reached a wall time reduction by a factor of 3000.

Together, the following four algorithm modifications enable this enormous speed up of the low-energy state search: (1) We focus on the best state hit within the SA run rather than on the final one; this is advantageous due to the non-equilibrium nature of SA. (2) Generalizing this idea, we stop the cooling process and restart it from the respective best-so-far state (without temperature change) an optimized number of times. (3) We determine the most appropriate initial and final temperatures of the exponential schedule used. (4) By means of OpenMP parallelization, we simultaneously perform only weakly interacting SA runs using 10 cores.

Although these ideas are rather obvious and, in part, have been used in various studies before, they seem to be not as widely known as they deserve to be. Therefore, we suggest to always include them in teaching SA, and to study the corresponding efficiency gain for further challenging optimization

problems.

An Improved Multicanonical Monte Carlo Algorithm for the Basis Expansion of the Density of States

Alfred Farris[1], Ying Wai Li[2], Markus Eisenbach[2]
[1]Center for Simulational Physics, The University of Georgia, Athens, USA. [2]National Center for Computational Sciences, Oak Ridge National Laboratory, Oak Ridge, USA

We propose an improved multicanonical Monte Carlo algorithm to obtain an analytic expression for the density of states (DOS) in the form of a basis set expansion. This algorithm is based on a recently developed scheme [1,2], which combines the advantages of previous algorithms such as Wang-Landau sampling [3] and multicanonical sampling [4]. By working with mathematical functions throughout the simulation, this method eliminates the need for histograms and thus bypasses the systematic error associated with discretizing continuous variables. In this extension, we introduce a two-step optimization procedure to improve the convergence of the DOS. As a test case, we apply this improved scheme to numerical integration as in [1,2]. We achieve agreement with Wang-Landau sampling while observing an order of magnitude speed-up. Moreover, the estimated DOS continuously improves with more samples without overfitting, and it converges in fewer iterations with much higher precision than the originally proposed algorithm.

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Efficient reduced density matrix functional theory with model interactions for solids

Johannes Voss
SLAC National Accelerator Laboratory, Menlo Park, USA

In reduced density matrix functional theory (RDMFT), many-electron ground states are expressed as functionals of the one-body reduced density matrix (1RDM). In contrast to the single Kohn-Sham Slater determinant approach of density functional theory, static correlation can be accounted for via fractional occupation eigenvalues of the 1RDM. Generally, minimization of an energy functional with a 1RDM-functional for exchange and correlation does not correspond to an eigenvalue problem for the natural orbitals, rendering the solution computationally challenging, unless the search is constrained to approximate orbitals satisfying effective single-particle Hamiltonians.

Here, a simple, explicitly orbital and occupation-dependent 1RDM exchange-correlation functional allowing for efficient solution via a self-consistent eigenvalue problem is presented. The simplicity of the functional is achieved by replacing Coulomb with model interactions, resulting in the same computational complexity as standard semi-local density functional theory. Benchmark results obtained with a plane wave implementation are shown, and limitations in the description of dimer dissociation due to the introduction of model interactions are discussed.

An Adaptive Wavelet Algorithm for Multi-Resolution Modeling in *n*-Dimensions with Error Control

Cale Harnish[1], Karel Matouš[1], Daniel Livescu[2]
[1]*University of Notre Dame, Notre Dame, USA.* [2]*Los Alamos National Laboratory, Los Alamos, USA*

The scale and complexity of practical engineering problems impose prohibitive computational requirements when using traditional numerical methods in multi-dimensional simulations. Algorithms must solve coupled systems of nonlinear partial differential equations (PDEs) with multi-physics features evolving on a wide range of spatial and temporal scales. To overcome these challenges, we have developed the Multi-Resolution Wavelet Toolkit (MRWT), an *n*-dimensional algorithm to solve PDEs with significant data compression and explicit error control.

MRWT exploits the multi-resolution nature of wavelet basis functions, and second generation wavelets, to solve initial-boundary value problems on finite domains. MRWT maximizes the traditional data compression of wavelets by projecting fields and spatial derivative operators onto the wavelet basis, and uses the minimum number of collocation points to define the coarsest resolution. We provide *a priori* error estimates for the wavelet representation of fields, their derivatives, and the aliasing errors associated with the nonlinear terms in a PDE. Then, our estimates are used to construct a sparse multi-resolution spatial discretization which guarantees the prescribed accuracy for each field. MRWT includes a predictor-corrector procedure within the time advancement loop to dynamically adapt the computational grid and maintain the prescribed accuracy of the solution of the PDE as it evolves. We have verified MRWT on nonlinear problems including Burgers' equation and the Navier-Stokes equations. Convergence to the analytical solutions is achieved at a rate which is in agreement with a priori estimates. Furthermore, we present an index notation for the wavelet operations to facilitate their extension to *n*-dimensional applications.

Wednesday, Parallel Sessions 1, 02:00PM-03:30PM

Materials 5

Conference Center, Ballroom A

Invited: How Materials Physics Drives Li-ion Battery Performance

Michelle Johannes[1], Noam Bernstein[1], Khang Hoang[2]
[1]Naval Research Laboratory, Washington, USA. [2]North Dakota State University, Fargo, USA

Although batteries are generally considered electrochemical systems, a surprising amount of their performance stems from the physics of the materials that make up their basic components: anode, cathode and electrolyte. Ionic conduction, electronic conductivity, chemical stability and voltage can all be traced back to intrinsic materials properties which are governed by fundamental physics.

In this talk, I will discuss how computational simulation can be used to gauge the utility of oxide and phosphate materials for use in Li-ion battery materials. More specifically, I will concentrate on the role of defects, which can be either highly beneficial, even essential, or strongly detrimental to necessary battery material properties. Using density functional theory, I will show how calculations can be used not only to provide a fundamental understanding of the relationship between materials properties and performance, but also to describe experimental conditions that lead to synthesis of better, optimized materials containing ”good” defects and lacking ”bad” ones. $LiMPO_4$ (M=transition metal) cathode materials and garnet structured oxide ($Li_7La_3Zr_2O_{12}$) solid electrolytes will be used as examples.

Invited: Enabling Large-Scale Physics Applications on Summit Through the Center for Accelerated Application Readiness

Jack Wells
Oak Ridge National Laboratory, USA

The Center for Accelerated Application Readiness (CAAR) within the Oak Ridge Leadership Computing Facility (OLCF) is a program to prepare scientific applications for next generation supercomputer architectures. Currently the program consists of thirteen domain science application development projects, including several in physics modeling and simulation, focusing on preparing codes for efficient use on Summit, the U.S. Department of Energy’s supercomputer deployed at OLCF in 2018. This presentation will highlight the progress made by CAAR teams and other early users on Summit in areas such as astrophysics, nuclear physics, lattice QCD, plasma physics, and materials physics. In addition, OLCF has realized recent growth in users focused on experimental and observational data analysis. Summit, with over 9,000 IBM Power 9 CPUs and over 27,000 NVIDIA GPUs integrated by high-bandwidth memory technologies, provides unprecedented opportunities to advance model-based simulation, machine learning, and data analytics.

Materials 6

Conference Center, Ballroom B

Invited: Spin Crossover in Lower Mantle Minerals

Renata Wentzcovitch
Columbia University, New York, USA

Pressure and temperature induced spin-state change in iron in lower mantle minerals is an unusual phenomenon with previously unknown consequences. High-pressure and high-temperature experiments have offered a wealth of new information about this class of materials problems, which includes the insulator to metal transition in Mott systems. I will discuss key experimental data, contrast them with our ab Initio results and thermodynamic models, show the implications for fundamental phenomena taking place at the atomic scale and their macroscopic manifestations, and discuss potential geophysical consequences of this phenomenon.

Invited: Predictive simulations of crystal plasticity: multiscale or cross-scale?

Vasily Bulatov
Lawrence Livermore National Laboratory, Livermore, USA

Prediction of crystal plasticity directly from the atomic motion has been regarded as impossible given the severe limits on time- and length-scale accessible to direct Molecular Dynamics (MD) simulations. The mesoscopic method of Discrete Dislocation Dynamics (DDD) was developed to bridge the wide scale gap and is now regarded as the principal method enabling such predictions. We will discuss a recently completed direct MD simulation of dislocation dynamics in which a single crystal of tantalum was compressed at rate 10^5/s. Referred to as Livermore BigBig (LBB) simulation, LBB is by far the largest MD simulation ever performed: it generated a dynamic trajectory of over 2.1 billion atoms over 5 microseconds of compressive straining. The simulation generated nearly 80 exabytes of recordable trajectory data a fraction of which was saved on disk in a highly compressed/post-processed form available for further analysis. As opposed to multiscale, LBB simulation can be regarded *cross-scale* being sufficiently large to be statistically representative of collective action of dislocations resulting in the macroscopic flow stress and yet fully resolved to every atomic "jiggle and wiggle". Importantly, LBB is sufficiently large to be used as a critical test of the mesoscopic DDD approach. To enable an "apples to apples" comparison, we calibrated our mesoscopic DDD model to match our atomistic LBB model at the level of single dislocation mobilities, shape and dimensions of the simulation volume, straining rate, temperature, straining axis, positioning and shape of initial dislocation sources, etc. Results of this comparison will be described.

Algorithms 1

Conference Center, Ballroom C

Invited: Quantum-driven classical optimization

Helmut G. Katzgraber
Texas A&M University, College Station, USA. 1QB Information Technologies, Vancouver, Canada

The advent of the first useful quantum computing devices has resulted in an arms race with classical algorithms on traditional computing hardware. While near-term quantum devices might revolutionize, e.g., optimization and quantum chemistry, tackling many applications will directly depend on either hybrid or purely classical computing techniques. Inspired by these recent exciting developments, a variety of new classical optimization techniques have emerged. In this talk an overview of quantum inspired methods, their application, as well as the current status on the classical-vs-quantum arms race is given. In particular, it is demonstrated how classical emulation of quantum mechanics can result in efficient optimization techniques on CMOS hardware.

Invited: The Question of Quantum Supremacy

Sergio Boixo[1], Vadim Smelyanskiy[1], Sergei Isakov[2], Charles Neill[3], Pedram Roushan[3], Kostya Kechedzhi[4], John Martinis[3], Hartmut Neven[1]
[1]Google, Venice, USA. [2]Google, Zurich, Switzerland. [3]Google, Santa Barbara, USA. [4]NASA, Ames, USA

We present a theoretical foundation for a practical demonstration of quantum supremacy in near-term devices: the task of sampling bit-strings from the output of random quantum circuits, which can be thought of as the "hello world" program for quantum computers. Arguably, this is the strongest theoretical proposal to prove an exponential separation between the computational power of classical and quantum computers. Determining where exactly the quantum supremacy frontier lies for sampling random quantum circuits has rapidly become an exciting area of research. On one hand, improvements in classical algorithms to simulate quantum circuits aim to increase the size of the quantum circuits required to establish quantum supremacy. This forces an experimental quantum device with a sufficiently large number of qubits and low enough error rates to implement circuits of sufficient depth (i.e the number of layers of gates in the circuit) to achieve supremacy. On the other hand, we now understand better how the particular choice of the quantum gates used to build random quantum circuits affects the simulation cost, leading to improved benchmarks for near-term quantum supremacy. We review several exagerated claims against near-term quantum supremacy. Sampling from random quantum circuits is also an excellent calibration benchmark for quantum computers, which we call cross-entropy benchmarking.

Wednesday, Parallel Sessions 2, 04:00PM-06:00PM

Software 3

Conference Center, Ballroom A

Minimally Invasive Adaptation of Computational Grids for Gyrokinetic Eulerian Simulations

Denis Jarema, Tobias Görler, Frank Jenko, Daniel Told
Max Planck Institute for Plasma Physics, Garching, Germany

The goal of fusion energy research is to mimic the Sun by confining a very hot hydrogen plasma in a donut-shaped magnetic field. The energy confinement time is controlled by turbulent transport in the fusion plasma, a process which can be studied on present-day supercomputers by means of (gyro-)kinetic simulations. Given that the plasma temperature often changes by 1-2 orders of magnitude between the hot core and the cold edge, the velocity-space discretization in grid-based methods needs to be spatially adapted for maximum efficiency. In this work, we address this issue by a grid-blocking technique. The new type of grids enhance the existing rectilinear grids in the heavily used grid-based code GENE (http://genecode.org). We also discuss how we accomplished a minimally invasive method that allows reusing the optimized implementation for the regular grids. Moreover, we demonstrate via several representative scenarios the achieved benefits: a significant reduction in the number of grid points, a high speedup, convergence of results like for the regular grids, a minimal computational overhead, as well as a reduced memory footprint and size of diagnostic data.

Heat Transport on Brownian Motors

Constancio Miguel Arizmendi[1], Karina Irma Mazzitello[1], Fereydoon Family[2]
[1]ICYTE, Facultad de Ingeniería, Universidad Nacional de Mar del Plata, Mar del Plata, Argentina. [2]Emory University, Atlanta, GA, USA

Thermal ratchets or Brownian motors achieve a net current of particles through thermal fluctuations rectification. The contact with one or several thermal baths is the source of thermal fluctuations. Brownian motors are kept away from equilibrium by external fluctuations or temperature gradients that make them completely different from Carnot engines. Studies on the Thermodynamics of these motors are mainly focused on efficiency. Nevertheless, high efficiency may be achieved with unintended heat dissipation. In this work we use a novel computational approach to elucidate the mechanism by which heat is dissipated to the thermal bath. The process of heat transport is related to the effective temperature through the generalization of the fluctuation–dissipation theorem on far from equilibrium systems. The effective temperature is defined by the comparison between induced and spontaneous fluctuations. We applied the replica method to the Brownian motor. Two replicas of the system with and without a perturbative force were computationally simulated to calculate the induced fluctuations and the response function. We found that the heat transport is different from Fourier´s Law and is proportional to the n_{th} power of the difference between the effective temperature of ratchet and the temperature of the bath. The power n depends only on the temperature of the bath. On the other hand the thermal conductivity depends on the bath temperature and also on both, the ratchet potential and the amplitude of the external source. In this way an expression of heat transport is obtained as a non-equilibrium measure.

A First Look at Lattice Effects in Coarse-Grained Protein Models via Wang-Landau Simulations

Alfred Farris[1], Daniel Seaton[2], **David Landau**[1]
[1]Center for Simulational Physics, The University of Georgia, Athens, USA. [2]Office for the Vice Provost for Advances in Learning, Harvard University, Cambridge, USA

In order to study the effects of lattice constraints on coarse-grained protein models, we apply Wang-Landau sampling [1] to the continuum analogue of the hydrophobic-polar (HP) lattice protein model [2]. The continuum version is inspired by the AB polymer model [3] but incorporates potentials tuned specifically to mimic those of the lattice case. Because of their relative simplicity, both the lattice and continuum models offer significant computational advantage over all-atom simulations (due to the simplified interactions and the reduction of the 20 amino acids to only two types), but the impact of the additional lattice constraint on generic folding behavior is unknown. In this study, we compare and contrast the behavior of thermodynamic and structural quantities during the folding process of the continuum model to the original HP lattice protein model [4] for sequences mapped from Crambin, a 46 amino acid plant protein. For both of these coarse-grained models, the folding process consists of multiple stages of collapse and reorganization.

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Analysis of Inhomogeneity: Brownian Dynamics Simulations of Tetra-Peg Gel Formation

Sayaka Waide[1], Hibiki Itoga[1], Ryota Morikawa[1], Takeshi Miyakawa[1], Takamasa Sakai[2], Ungil Chung[2], **Masako Takasu**[1]
[1]Tokyo Univ. of Pharm. and Life Sciences, Tokyo, Japan. [2]Univ. of Tokyo, Tokyo, Japan

Tetra-PEG is a monomer which has four arms and functional group in each terminal of the arm. For modeling Tetra-PEG gel [1], we used a coarse-grained model including five particles and four bonds. If the distance of the terminals of different molecules is smaller than the threshold value, a bond is generated between the terminals. We performed Brownian Dynamics simulations for the model, and calculated the gel formation process. To investigate the inhomogeneity, we evaluated the distribution of the length of the branch, and also the distribution of the volume of Voronoi cell for each molecule, branch and cluster. When the monomer density is high, inhomogeneity for length of the branch and also for volume of monomer and branch decrease.

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Modelling of stochastic transport problems using exclusion processes

Atul Kumar Verma, Arvind Kumar Gupta
Department of Mathematics, IIT Ropar, India-140001, Ropar, India

Many natural systems exhibit complex behaviour under the stationary state when either driven by some external field or self-driven. Such driven diffusive systems reveal very rich nonequilibrium phenomena in physics, chemistry and biology such as kinetics of bio-polymerization dynamics of motor proteins in biological cells, gel electrophoresis, vehicular traffic and modelling of ant-trails. In biological systems, molecular motors are motor proteins that consume chemical energy and move along polymer filaments of the cytoskeleton, which act as macromolecular tracks. Their collective dynamics plays a major role in various intracellular processes/functions such as cellular trafficking, protein synthesis, cell division etc. In order to analyze the collective properties of interacting molecular motors and other driven stochastic transport problems, totally asymmetrically simple exclusion process (TASEP) model that is an out of equilibrium system is found to be a paradigmatic model to study such problems in the last decade. TASEP model comprises of single species of particles performing biased hopping with the uniform rate in a preferred direction along a 1D lattice. The particles obey certain preassigned rules under hard-core exclusion principle, due to which a lattice site cannot have more than one particle.

In this work, we have tried to analyze the intracellular and vehicular transport systems along multiple highways using a three-channel TASEP with the attachment-detachment process. The steady-state theoretical results are verified by extensively performed Monte Carlo simulations.

Overcoming the Carbuncle Instability for the HLLC-type Riemann Solver

Zhijun Shen, Xia Cui
Institute of Applied Physics and Computational Mathematics, Beijing, China

The carbuncle phenomenon is a shock instability mechanism which may ruin all efforts to compute grid-aligned shock waves using low-dissipative upwind schemes. This research investigates solution behaviors of the HLLC-type methods for the Euler equations under the strong shock interaction and strategies to cure shock instability; here the HLLC-type methods include HLLEM [1], HLLCM [2] and other Riemann solvers [3] with contact wave exactly. Based on a matrix stability analysis for two dimensional steady shock [4, 5], some new factors to influence carbuncle phenomenon are pointed out, such as the way of wave velocity estimates. A suggestion to the choice of wave speed is proposed when calculating strong shock wave problems.

It is well known that the shear viscosity is a very important factor to suppress numerical instability phenomenon. Implementing appropriate shear viscosity is a crucial way to improve computation effect. Another work here is to quantify the amount of suppression needed in the shear wave when problems with a given Mach number are handled. The purpose is to provide indiscipline scientist or engineer some helps to overcome the pathologies when simulating related problems.

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Viscoelastic Flow With Partial Slip Through a Two Heated Plate Influenced by Magnetic Field

Umar Bala, Mijinyawa Sani Labaran, Mohammed Abdulhameed
Federal Polytechnic, Bauchi, Bauchi State, Nigeria

In this paper, based on magnetohydrodynamic (MHD) approach, the viscoelastic fluid flow with patial slip through a two heated parallel plate was studied. The heat transfer on prescribed temperature was also considered. The coupled non-linear differential equations arising from the model are solved using ananlytical techniques. For hydrodynamic (HD) flow, the present results momentum equation are found to be analytically identical to those of published work. Effects of thermophysical parameters are analyzed and potrayed graphically.

Key words: Partial slip, MHD flow, Fourth order fluid, Heat transfer, Analytical solutions

Materials 7

Conference Center, Ballroom B

Classification of Atomic Environments using the Gromov-Wasserstein Distance

Jeremy Mason[1], Benjamin Schweinhart[2]
[1]University of California, Davis, Davis, USA. [2]Ohio State University, Columbus, USA

Contemporary molecular dynamics simulations often contain many millions of atoms, and automated classification of local atomic environments is increasingly necessary to process the data generated by these simulations. Previous approaches, such as the centrosymmtery parameter and common neighbor analysis, can fail to distinguish between certain solid phases or lack important mathematical properties such as stability with respect to small perturbations. We propose the 1-Gromov-Wassertein distance as an alternative method to classify local atomic environments. We use this distance to identify defects in a simulation of a polycrystalline material, and compare its ability to distinguish distinct phases to several methods previously proposed in the literature.

Discovering a Novel Nanometric Cubic Phase in Monochalcogenide Semiconductors – The Critical Role of Adsorbed Ligands

Elad Segev[1], Ran Eitan Abutbul[1,2], Uri Argaman[2], Yuval Golan[1,2], Guy Makov[1,2]
[1]Ben-Gurion University of the Negev, Ilse Katz Institute for Nanoscale Science and Technology, Beer-Sheva, Israel. [2]Ben-Gurion University of the Negev, Department of Materials Engineering, Beer-Sheva, Israel

A new nanometric cubic binary phase was recently discovered in tin monosulfide. However, its identification and characterization proved challenging and was confirmed by a combination of experimental and theoretical modelling to be a previously unknown, low symmetry 64-atom cubic structure. Subsequently, this phase was synthesized and identified in tin monoselenide and posited to exist in germanium monosulfide and monoselenide based on density functional theory calculations. A series of computational and experimental studies have identified promising optical properties due to the larger bandgap and non-centrosymmetric structure of the crystal. The structure, atomic positions and band gaps of these phases were determined by ab-initio density functional calculations and found to be in very good agreement with experimental measurements. The phases were determined to be mechanically stable and energetically close to competing structures such as rhombohedral and orthorhombic. Surface energy calculations indicate that the particles must be stabilized by ligands adsorption the properties of which are being explored and may explain the nanocrystals growth mechanism. This talk will focus on the results of our calculations of surface energies and the effects of different ligand molecules adsorbed, and their interplay with experimental studies.

Ultraflat bands and shear solitons in Moiré patterns of twisted bilayer transition metal dichalcogenides.

Mit H. Naik, Manish Jain
Indian Institute of Science, Bangalore, India

Ultraflat bands in twisted bilayers of two-dimensional materials have a strong potential to host strongly-

correlated phases. Using first principles density functional theory calculations, we show the emergence of ultraflat bands at the valence band edge in twisted bilayer MoS_2, a prototypical transition metal dichalcogenide. The computed band widths, 5 meV and 15 meV for 56.5° and 3.5° twist angles respectively, are comparable to that of twisted bilayer graphene near 'magic' angles. Large structural transformations in the Moiré patterns lead to formation of shear solitons at stacking boundaries and strongly influence the electronic structure. We extend our analysis for twisted bilayer MoS_2 to show that flat bands can occur at the valence band edge of twisted bilayer WS_2, $MoSe_2$ and WSe_2 as well.

Density Functional Theory Studies of Graphene/Sodium Oxide Composites

Regina Maphanga[1], Nicola Seriani[2]
[1]Council for Scientific and Industrial Research, Pretoria, South Africa. [2]ICTP, Trieste, Italy

The ever-increasing global energy needs and depleting fossil-fuel resources demand the pursuit of sustainable energy alternatives, including both renewable energy sources and sustainable storage technologies. The high electrochemical theoretical specific capacity, specific capacitance and ultra large surface-to volume ratio, when combined with its remarkable properties, make graphene an ideal material for enhanced energy storage particularly in batteries. Chemically derived graphene suffers from agglomeration and restacking after removal of dispersed solutions and drying due to the van der Waals interactions. Therefore, graphene/metal oxide composites offer a combined advantages of both graphene and metal oxides as active materials for improving the electrochemical energy storage and solve problems associated with the individual components of graphene or metal oxides. In this paper, reaction mechanisms of graphene/sodium oxide composites are investigated using generalized gradient approximation implemented in density functional theory. Variation on Na_xO_y adsorption sites relative to two adjacent carbon atoms and high symmetry hollow point for oxygen and sodium atoms respectively is considered. All considered adsorption sites revealed that adsorbent molecules move away from graphene layer together with two adjacent carbons aligned to oxygen atoms, suggesting a formation of a bond between C and O atoms, most likely to form Na_2CO_3product. Sodium superoxide NaO_2 was found to be more likely to form than other sodium oxides (NaO, Na_2O and Na_2O_2) in Na-air batteries. In contrast, analogous Li_2O_2 is thermodynamically favourable in the case of Li-air batteries.

Microscopic behavior of hydrogen on PuO_2(110) surfaces from first principles calculations

Huilong Yu
Insititute of Materials, China Academy of Engineering Physics, JIANGYOU, China

Plutonium is an important nuclear material in some nuclear reactors as a source of energy. It is a chemically reactive metal. Plutonium shows enormous and reversible reaction rates exposed to hydrogen. The safe handling and storage of plutonium metal requires an understanding of plutonium corrosion by hydrogen. In the presence of air or oxygen, plutonium metal surface rapidly becomes covered with PuO_2, which may be exposed to hydrogen atmosphere during plutonium handling and long storage process. It is the key factor of the reaction between plutonium and hydrogen. The adsorption, dissociation and diffusion of hydrogen on PuO_2 (110) surface have been investigated by GGA+U. In order to find out the energetically more favorable adsorption site, optimum dissociation and diffusion path, adsorption energy of hydrogen on various sites, the dissociation and diffusion energy barrier are de-

rived and compared. The results show that H_2 molecules are weakly adsorbed on PuO_2 (110) surface, while H atoms are strongly bonded at the top of O atom sites. One possible dissociation pathway of H_2 molecule is investigated using the cNEB approach. The calculated barriers show that the dissociation of H_2 molecule on PuO_2 (110) surface is kinetically the most favorable and can occur even below room temperature. Atomic H diffusion from surface to subsurface is investigated, the results indicate that it is energetically more favorable for H atom to be on the surface. Hydrogen permeation through purity PuO_2 surface is mainly inhibited from hydrogen atom diffusion from surface to subsurface.

Ab Initio Investigation of Nanotribological Properties of the Hexagonal BN/Au(111) Interface

Merve Baksi[1], Oğuz Gülseren[2], Hande Toffoli[1]
[1]Middle East Technical University, Ankara, Turkey. [2]Bilkent University, Ankara, Turkey

As the size of the systems reduces due to advances in fabrication techniques, materials properties that apply at macroscopic scale start to lose their validity. As a reflection of this, friction at the atomic scale does not obey the macroscopic Da Vinci-Amontons' description [1]. Each interface that experiences losses due to friction therefore requires a separate examination. A particularly intensely studied class of materials from a nanotribological point of view is two-dimensional networks. In addition to the interface of two-dimensional materials with themselves, the interface between these materials and bulk surfaces are of interest.

In this work, we report nanotribological properties of h-BN/h-BN (hexagonal boron nitride), and h-BN/Au(111) surfaces using Density Functional Theory (DFT). h-BN is a wide band-gap semiconductor with the same hexagonal honeycomb lattice as graphene. We first report our calculated lateral friction forces and friction coefficients of h-BN/h-BN interface when they are in relative motion. We then report similar results for h-BN/Au(111) interface. The latter calculations are particularly relevant for modelling friction force microscopy experiments [2]. We identify and discuss trends in the behavior of friction force as a function of vertical load and for experimentally feasible contact areas. Furthermore, to understand the effects of the edges of the interface, we also investigate the interaction between small Au clusters and h-BN network.

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I-V Characteristics of In-Plate Graphene Nanoribbon/h-BN Heterojunctions and Resonant Tunneling

Mitsuyoshi Tomiya, Taiga Wakai, Shoichi Sakamoto
Seikei Univeristy, 3-3-1 Kichijoji-Kitamachi, Musashino-shi, Tokyo 180-8633, Japan

We present the first principle calculations of the electrical properties of in-plate heterojunctions of graphene sheet/h-BN(GS/h-BN), armchair graphene nanoribbon/h-BN(AGNR/h-BN), and zigzag graphene nanoribbon/h-BN which are carried out using SIESTA package, which is comprised of numerical codes of the density functional theory(DFT) and the non-equilibrium Green's function(NEGF). Especially, adopting the conductive (3n-1)-family of AGNR, the lead parts in both side of the model become metallic. Two transverse arrays of h-BN, which is a wide-gap semi-conductor, are embedded in the middle of sheet/nanoribbon and act as a double barrier system.

The quantum double barrier tunneling is found in the transmission functions(TF) and I-V characteristics of GS/h-BN and 11-AGNR/h-BN. The TF shows very spiky peaks in a neighborhood of the Fermi energy, and consequently, I-V characteristics becomes step-wise. Simple one-dimensional Dirac equation model for the double barrier system is also proposed to analyze numerical results. Our model reproduces most of the peaks of the transmission functions nearby the Fermi energy, as a result of quantum tunneling.

Algorithms 2

Conference Center, Ballroom C

Phase diagram of six-state clock model on rewired square lattices

Tasrief Surungan
Hasanuddin University, Makassar, Indonesia

The six-state clock model (SSCM) on rewired square lattice is studied via Monte Carlo simulation with Wang-Landau algorithm. This is a discrete counterpart of the XY model with a unique topological phase transition called Kosterlitz-Tholess (KT) transition. The model has two KT transitions, i.e., at temperature T_1 and T_2, where $T_1 < T_2$. The first transition separates the magnetic order and the quasi-long range order (QLRO) also known as KT phase; while the second transition separates the QLRO and the paramagnetic phase. It was reported that the presence of KT phase is affected by the presence of randomness in the form of site and bond dilution. This intermediate phase is totally ruled out if bonds or sites of the lattice are no longer percolated. Here we probe different type of randomness, namely by rewiring the lattice. We randomly add one or two extra bonds to each lattice site, and connect the site to its second or third nearest neighbors. As a results, the average number of neighbors C increases. The increase of C affects the existence of KT phase. For each value of C, we calculate the correlation ratio for detecting and analyzing the existing the KT phase. Variation of KT temperatures (T_1 and T_2) for different values of C is observed, which is plotted with respect to each corresponding C to obtain the system phase diagram.

DCA++ project: Sustainable and scalable development of a high-performance research code

Urs R. Hähner[1], Peter W. Doak[2], Thomas A. Maier[2], Raffaele Solcà[3], Thomas C. Schulthess[1,3]
[1]Institute for Theoretical Physics, ETH Zurich, Zurich, Switzerland. [2]Computational Science and Engineering Division and Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, USA. [3]Swiss National Supercomputing Center, ETH Zurich, Lugano, Switzerland

Scientific discoveries across all fields, from physics to biology, are increasingly driven by computer simulations. At the same time, the computational demand of many problems necessitates large-scale calculations on high-performance supercomputers. Developing and maintaining the underlying codes, however, has become a challenging task due to a combination of multiple factors. Leadership computer systems require massive parallelism, while the diversity of architectures needs to be abstracted away by a generic programming model. New sophisticated algorithms are continuously developed and have to be implemented in such complex environment. Finally, the multidisciplinary nature of modern science demands large, changing teams to work on a given code base. We use the DCA++ project, which develops a highly scalable and efficient research code to solve strongly correlated electron problems with cutting edge algorithms, to explore how scientific software development can overcome these challenges. We show how best practices in software engineering can be applied to make software development in a research group sustainable and how performance sensitive codes can be developed in close collaboration with experts from HPC centers.

QuSP: The Quantum Simulator Package

Matthew Jones[1,2], Daniel Jaschke[1], Lincoln Carr[1]
[1]Colorado School of Mines, Golden, USA. [2]Nvidia Corporation, Santa Clara, USA

Here, we present a new computational tool to facilitate the design of quantum computing technologies: QuSP, The Quantum Simulator Package. Backed with a modular library base with an extensible, easy-to-use API, and fronted with a simple GUI, QuSP seeks to enable the application of quantum physics to technology.

With its ability to intelligently spin up simulations, back them with free HPC resources, and dynamically visualize the output, QuSP provides users with an end-to-end solution for designing physical systems with purpose. Combine this with its low-level features, and QuSP presents value to developers at all stages.

Given its opensource genealogy, customizeable deployments of QuSP form a key design consideration with complete support.

With a focus on open quantum mechanically entangled many body systems, long range interactions, and decoherence, QuSP seeks to address outstanding questions and emergent phenomena in the field of quantum complexity.

As a package, QuSP includes

- Methods for
  - Exact Diagonalization
  - Matrix Product States, TEBD, DRMG, etc.
  - Matrix Product Operators, density matrix formalism
  - Unitary time evolution, Lindblad Master Equation, and more
  - Quantum Trajectories

- Models for
  - Ising, Hubbard, Heisenberg, XYZ
  - Quantum Cellular Automata
  - Nanoribbons, disorder, scattering, quantum coherent FETs

With support from the Science Gateways Community Institute, QuSP hopes to address a need for an extensible, easy-to-use tool to facilitate innovation in the area of quantum technologies design.

QuSP is based on OpenMPS (also known as OSMPS), which can be found here:

https://sourceforge.net/projects/openmps/

Alkyl group functionalization–induced thermal conductivity attenuation in graphene nanoribbons

Lu Shuang, Yu Xiaodong, **Li Haipeng**
School of Physical Science and Technology, China University of Mining and Technology, Xuzhou, China

We calculated the room temperature phonon thermal conductivity and phonon spectrum of alky group functionalized graphene nanoribbions (GNRs) with molecular dynamics simulations. It is found that the

increase of length and concentration of alkyl groups can cause remarkable reduction of thermal conductivity in functionalized GNRs. In addition, the alkyl group functionalization induces silightly change in the low frequency acoustic modes while significently suppresses the high frequency optical mode due to the remarkable phonons–structural defects scattering effect. We found that the phonon thermal conductivity attenuation in alkyl group functionalizaed GNR is mainly attributed to a reduction of the phonon mean free path induced by phonon–structural defects scaterring. Our study shows that surface functionalization is an effective routine to tune the phonon thermal conductivity of GNRs, which is very usefu to the graphene thermal–related applications including thermal management and thermoelectrics.

Electronic Stopping as a Function of Local DensityElectronic Stopping as a Function of Local Density

Artur Tamm[1], Magdalena Caro[2], Alfredo Caro[3], Alfredo Correa[1]
[1]Lawrence Livermore National Laboratory, Livermore, USA. [2]Virginia Polytechnic Institute, Arlington, USA. [3]George Washington University, Ashburn, USA

We present a model to capture electronic stopping within classical molecular dynamics (MD) based on ab initio calculations. Non-adiabatic time-dependent density functional theory (TDDFT) calculations provide a way to obtain the detailed behaviour of the energy dissipation by an energetic projectile in a host crystal at the atomistic level. Nevertheless, this ab initio method is computationally expensive and can only be applied to sample containing a small amount of atoms. Therefore, a need for a model to reproduce the captured physics within classical MD arises. Previously we have shown that our model based on spatial correlations is able to capture the main trends of electron-phonon coupling in classical MD simulations. In a semiclassical picture, electronic stopping power and electron-phonon interaction are fundamentally linked, this model could be used to incorporate the electronic effects of both phenomena simultaneously. We show the applicability of our model to capture such effects in the example of a Ni FCC crystal. Our resulting model shows that the average energy transfer due to electronic stopping is comparable to the TDDFT results along various trajectories. The proposed model could be of great importance in the collision cascade simulations, which can only be realised with classical MD. Finally, our model is readily applicable to alloys.

Prepared by LLNL under Contract DE-AC52-07NA27344

LLNL-ABS-749408

Charge equilibration and electronic stopping for silicon projectiles in silicon

Cheng-Wei Lee, Andre Schleife
University of Illinois, Urbana-Champaign, Urbana, USA

Charged energetic particle radiation has technological interest in applications including nuclear energy, outer space, medicine, and fundamental research. As a result of the irradiation, damage, like point defects, form and ultimately determine the material properties. Therefore, understanding the underlying interaction between charged particles and a material from first principles is important. Previously, we successfully used Ehrenfest molecular dynamics and real-time time-dependent density functional theory (RT-TDDFT) to describe electronic stopping for light projectiles during the early stages of radiation damage. Recently, we investigated heavy (silicon) projectiles traversing silicon bulk crystals and found a pronounced dependence of electronic stopping on the initial condition, which is not observed for light

projectiles. Here we analyze these recent results in terms of dynamics of charge equilibration, choices of trajectory (impact parameter), and contributions of core and valence electrons to electronic stopping. We demonstrate that off-channeling trajectories as well as semi-core electrons are needed for a direct comparison to experiment. These effects can be accurately predicted by RT-TDDFT. We also illustrate that developing a consistent framework based on first principles is an essential part of a multi-scale simulation approach that can accurately predict damage formation after particle irradiation.

Thursday, Parallel Sessions 1, 02:00PM-03:30PM

Soft Matter 1

Conference Center, Ballroom A

Invited: Enhanced sampling methods for spin systems and biomolecular systems

Yuko Okamoto
Nagoya University, Nagoya, Japan

Conventional Monte Carlo and molecular dynamics simulations are greatly hampered by the multiple-minima problem, where the simulations tend to get trapped in some of astronomically large number of local-minimum energy states. In order to overcome this difficulty, we have been advocating the uses of generalized-ensemble algorithms which are based on non-Boltzmann weight factors. With these algorithms we can explore a wide range of the conformational space. The advantage of generalized-ensemble algorithms such as replica-exchange method (or, parallel tempering) lies in the fact that from only one simulation run, one can obtain various thermodynamic quantities as functions of temperature and other physical parameters by the reweighting techniques. In this talk, I will present the latest results of various applications of generalized-ensemble algorithms to spin systems and biomolecular systems.

Mechanisms of Antimicrobial Peptide-Induced Vesicle Shape Transformation and Pore Formation

Lianghui Gao Gao, Yu Shi, Mingwei Wan
College of Chemistry, Beijing Normal University, Beijing, China

Pore-forming antimicrobial peptides not only create holes in bacterial membrane that allow leakage of cytoplasmic components, but also induce surface corrugation and surface-bound vesiculation. It is unclear whether the same or different chemical and physical effects determine the rich pepide-induced cell morphological and shape changes and the final cell death. In this study, we present coarse-grained molecular dynamics simulations of pore-forming antimicrobial peptide Melittin interacting with vesicles composed of mixture of zwitterionic and anionic phospholipids. We find that the adsorption of Melittin induces vesicle budding that can develop into vesiculation at high peptide concentration, and vesicle invagination that can eventually result in corrugated membrane surface. We demonstrate that these rich morphology changes are mediated by vesicles curvature and peptide concentration. Highly curved vesicles favor to recruit Melittins with a higher density of binding sites. The peptides mainly penetrate into the membrane surface in monomers via hydrophobic interaction. Lowly curved vesicles recruit Melittins with a low density of binding sites. Surplus peptides are prone to form oligomers and shallowly adsorb on the surface of the membrane via electrostatic interaction. The penetration of monomers induces membrane pore formation and positive membrane curvature that promotes vesicle budding, while the adsorption of oligomers induces negative membrane curvature that promotes vesicle invagination.

Dynamics of Viral Mutation and Evolution

Barbara Jones[1], Greyson Lewis[2], Wallace Marshall[2]
[1]IBM Research - Almaden, San Jose, USA. [2]Dept of Biochemistry and Biophysics, UCSF, San Francisco, USA

We study a model of viral evolution, in which viruses have a barrier to cell entry, mediated by their match to cell ”key”, followed by a viral-type dependent immune response by the cell, and finally a probability to reproduce and mutate. These mutated viruses then go on to attack other cells in the model. Previously we found equilibrium behavior, featuring a phase transition as a function of temperature and immunity [PLOS One 2015 https://doi.org/10.1371/journal.pone.0137482]. Here we describe our computational studies of the behavior of this model as a dynamical system, and the nonequilibrium evolution of the quasispecies distribution including metastable states and other unexpected features.

Effect of varying environmental conditions on the conformation change of a protein

Sunita Negi
Amity University, Gurgaon, India

The response of a protein is majorly dependent on the environmental conditions surrounding it. In this work we study the behavior of Calmodulin (CaM) protein as a function of its calcium ion concentration and ionic strength of the solution surrounding it. These studies are performed using extensive classical molecular dynamics simulations using NAMD software. As expected the protein is observed to acquire more flexibility as the calcium ions are loosened from its initial protein data bank (PDB) structure. The flexibility of the protein is observed to increase as the ionic strength of the solution is increased. This could be because of the strong ionic interactions between the charged residues of the protein and the ions in the solution. We expect the same kind of behavior from the other proteins as well indicating the calcium ion concentration and ionic strength of the surrounding solution as the key role players in the confirmation change of the protein.

Materials 8

Conference Center, Ballroom B

Invited: Fermi-Löwdin orbital self-interaction correction: efficient density functional theory calculations without self-interaction

Koblar Jackson
Central Michigan University, Mt. Pleasant, MI, USA

Density Functional Theory (DFT) is the method of choice for the atomistic modeling of materials. Modern density functionals achieve remarkable accuracy in describing properties when atoms are near their equilibrium positions, yet all semi-local functionals are subject to self-interaction errors that appear in stretched-bond situations and in many cases involving, for example, charge transfer. The Fermi-Löwdin orbital self-interaction correction or FLOSIC method was developed[1] to remove such errors efficiently by implementing the Perdew-Zunger self-interaction correction (PZ-SIC) without imposing computationally costly constraints. In this talk we outline the FLOSIC formalism and present the results of several recent calculations[2,3] that demonstrate its performance in removing self-interaction errors in practical calculations. In particular, we show that FLOSIC: i) shifts orbital energies to bring them into better agreement with experimental removal energies; ii) improves the description of magnetic exchange couplings; and iii) removes delocalization errors that lead to unphysical molecular dissociation. Finally, we discuss the outlook for combining FLOSIC with sophisticated density functionals to deliver efficient and accurate density functional calculations in all situations without self-interaction.

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On the interface tension of the Ising model

Elmar Bittner[1], Andreas Nussbaumer[2]
[1]ITP, Heidelberg University, Heidelberg, Germany. [2]Institute of Physics, JGU Mainz, Mainz, Germany

We determine the interface tension for the two and three dimensional Ising model using multicanonical simulations. We analyse the finite-size scaling behaviour of the interface tension for various temperatures, and compare them to previous results obtained with a combination of the multimagnetic algorithm with the parallel tempering method. We also use exact finite-size scaling functions for the two dimensional Ising model to validate our results.

Adaptive population Monte Carlo simulations

Martin Weigel[1], Lev Barash[2], Lev Shchur[2], Wolfhard Janke[3]
[1]Coventry University, Coventry, Germany. [2]Landau Institute for Theoretical Physics, Chernogolovka, Russian Federation. [3]Leipzig University, Leipzig, Germany

Population annealing is a sequential Monte Carlo scheme that is potentially able to make use of highly parallel computational resources. Additionally, it promises to allow for the accelerated simulation of systems with complex free-energy landscapes, much alike to the much more well known replica-exchange

or parallel tempering approach. We equip this method with self-adaptive and machine learning schemes for choosing the algorithmic parameters, including the temperature and sweep protocols as well as the population size. The resulting method is significantly more efficient for simulations of systems with complex free-energy landscapes than some more traditional approaches, and it is particularly well suited for massively parallel computing environments such as (clusters of) GPUs.

Large Deviations of Convex Hulls of Self-Avoiding Random Walks

Hendrik Schawe[1], Alexander K. Hartmann[1], Satya N. Majumdar[2]
[1]*Universität Oldenburg, Oldenburg, Germany.* [2]*LPTMS, Univ. Paris-Sud, Orsay, France*

A global picture of a random particle movement is given by the convex hull of the visited points. We obtained numerically the probability distributions of the volume and surface of the convex hulls of a selection of self-avoiding random walks, e.g., the classical self-avoiding walk and the loop erased walk. To obtain a comprehensive description of the measured random quantities, we applied sophisticated large-deviation techniques, which allowed us to obtain the distributions over a large range of the support down to probabilities far smaller than $P = 10^{-100}$. We give an approximate closed form of the so-called large-deviation rate function Φ which generalizes above the upper critical dimension to the previously studied case of the standard random walk.

Quantum Many-body 3

Conference Center, Ballroom C

Invited: Quantum Monte Carlo investigations of correlated electron systems, present and future

Zi Yang Meng

Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Beijing, China

In this talk, I will present recent developments in conceptual and technical aspects of numerical simulations in correlated electron systems, in particular in the new quantum Monte Carlo methods. Fresh results on itinerant quantum critical points, i.e. the critical phenomena arising from the strong coupling between Fermi surface and bosonic fluctuations will be discussed, as well as the recently discovered, fundamental duality relations between interaction-driven topological phase transitions and deconfined quantum critical points. For the latter, not only its static but also dynamical properties, are revealed via unbiased large-scale numerical efforts. In the end, I will point out promising future directions in combining numerical methods and quantum field theory in the era of big-data and artificial intelligence in pursuing the understanding of correlated electron systems.

References:

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A computational framework for model Hamiltonian construction from materials properties

Ying Wai Li[1], Anjana Samarakoon[1], Markus Eisenbach[1], Kipton Barros[2], Hidemaro Suwa[3], Cristian Batista[3], Alan Tennant[1]

[1]*Oak Ridge National Laboratory, Oak Ridge, USA.* [2]*Los Alamos National Laboratory, Los Alamos, USA.* [3]*University of Tennessee, Knoxville, Knoxville, USA*

In the theoretical study of material properties, model Hamiltonians play a crucial role to understand physical interactions that account for materials behavior and observables. Some of these properties can be measured by experiments directly, such as the static and dynamical structure factors from neutron scattering. These physical observables hence serve as the middle ground for matching theoretical predictions and experimental measurements. However, establishing such a connection, i.e., identifying minimal model Hamiltonians that provide theoretical explanations of the observed data, is a challenging problem in materials science. One of the reasons is that it is an inverse problem in a large search space of high-dimensional parameters, in addition to fitting to a large amount of experimental data. Here, we present a computational framework that applies optimization and machine learning techniques to construct model Hamiltonians directly from experimental data. We devise an automated, iterative procedure that surveys the model space efficiently to refine the model parameters until convergence. Our preliminary results indicate that this novel computational scheme will be able to drive the theoretical understanding of materials from advanced analytics of experimental data.

Fluctuating stripes in Hubbard models of high-T_c cuprate superconductors

Brian Moritz[1,2], Edwin W. Huang[2], Hong-Chen Jiang[1,2], Thomas P. Devereaux[1,2]
[1]*SLAC National Accelerator Laboratory, Menlo Park, USA.* [2]*Stanford University, Stanford, USA*

Microscopic models designed to capture the strongly correlated physics embodied in the cuprates must accurately reflect the translational and rotational symmetry breaking present in the form of stripes. We investigate the emergence of these stripes in single and multi-orbital Hubbard models, using determinant quantum Monte Carlo (DQMC) simulations at finite temperatures, and compare with density matrix renormalization group (DMRG) results at zero temperature. Our analysis reveals the presence of fluctuating spin stripes at high temperatures in these models, over a significant range of doping, temperatures, and variations in other model parameters appropriate to the cuprates. We naturally capture the absence of spin stripes in electron-doped materials and find nearly half-filled stripes upon hole-doping. The similarities between our results and experiments support a unified description of fluctuating stripes across a large portion of the cuprate phase diagram.

Time-evolution of optical excitations in Fe/MgO(001) superlattice from RT-TDDFT

Markus Ernst Gruner, **Rossitza Pentcheva**
University of Duisburg-Essen, Duisburg, Germany

We investigate the real-time (RT) evolution of an optical excitation in a $(Fe)_n/(MgO)_m(001)$ multilayer system in the framework of time-dependent density functional theory (TDDFT). The calculations are carried out with the ELK code using the adiabatic local spin density approximation for exchange and correlation. Starting with a minimum model consisting of a single Fe layer and 3 MgO layers, we vary systematically frequency and fluence of the laser pulse and analyze the time-dependent propagation of excitations in terms of the variation of the charge density and electronic density of states, which gives insight into the evolution of orbital polarisation. Apart from laser frequency and intensity, we find that also the polarization of light significantly influences the magnitude and propagation of the excitations.

Financial support from the DFG within SFB 1242 (project C02) and computational time at magnitUDE is gratefully acknowledged.

Thursday, Parallel Sessions 2, 04:00PM-06:00PM

Soft Matter 2

Conference Center, Ballroom A

Thermodynamic and Structural Similarity of Crambin Lattice Protein Homologues

Zewen Zhang[1], Alfred Farris[1], Thomas Wüst[2], Guangjie Shi[1], David Landau[1]
[1]Center for Simulational Physics, University of Georgia, Athens, USA. [2]Scientific IT Services, ETH Zürich, Zürich, Switzerland

The H0P lattice protein model is an extension of the HP model 1 with an extra third kind of "neutral" monomer. As a widely-used prototype, Crambin (a 46 amino acids protein) has been mapped onto the H0P model and studied by replica-exchange Wang-Landau sampling 2. From this, we obtain the density of states and are able to extract thermal properties of the lattice protein at all temperature. With further study by multicanonical sampling, ground states as well as the temperature-dependence of structural quantities are measured with high resolution 3. In this study, we examine five H0P lattice protein homologues of Crambin, i.e. proteins with similar sequences and structures in nature. Our results show that, at low temperature, thermal properties of these homologues are close to those of Crambin itself, all showing two significant conformational changes around the same temperature. However, the structural quantities (e.g. end-to-end distance) look very different for Crambin and its homologues, which implies that the structural similarity among these tested lattice proteins is relatively low.

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Predicted pathways for chemical degradation in siloxane polymers following phenyl excitations

Matthew Kroonblawd[1], Nir Goldman[1,2], James Lewicki[1]
[1]Lawrence Livermore National Laboratory, Livermore, USA. [2]University of California, Davis, USA

Chemical degradation processes can result in undesirable changes in the performance of functional materials over the service lifetime. Detailed characterizations of such phenomena are critical for understanding material aging, but atomic-scale chemical processes are often subtle to probe. Molecular dynamics using semiempirical quantum models provides an accurate and efficient approach to predict condensed-phase chemistry that is difficult to elucidate from experiments alone.We investigate the initial steps of benzene off-gassing in a model polydimethylsiloxane (PDMS) and polydiphenylsiloxane (PDPS) copolymer system using the semiempirical density functional tight binding approach. Accelerated simulation approaches are combined with an ensemble methodology to sample dephenylation processes in a variety of compressed and stretched polymeric strands. Our simulations reveal complicated reaction pathways including strand scissions, cyclizations, and the formation of polyphenyl moieties. Influence of environmental factors such as humidity on the resulting chemistry are discussed. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

It May be Possible to construct a “Reversible” Computer out of Capillary Tubes

Richard Kriske

Several years ago this Author proposed that Capillary Action Could be used to construct a Computer. It may not be useful to anything, except plants, but it may shine some light on the inner workings of plants, and how it is they are able to move, to synthesize and to adapt to their environments. This author had previously suggested that Capillary action, may in fact be a simple machine of Quantum Mechanics in much the same way that the Ramp, Lever and Pulley are the simple machines of Classical Mechanics.

Charge transport in branched conducting polymers: Quantum graphs based approach

Doniyor Babajanov[1], Hikmat Matyoqubov[2]
[1]Turin Polytechnic University in Tashkent, Tashkent, Uzbekistan. [2]Urgench State University, Urgench, Uzbekistan

Conducting polymers has attracted much attention recently in the context of organic electronics. Some types of such polymers can have supramolecular (macroscopic) branching.

Branched polymers occur when groups of units branch off from the long polymer chain. These branches are known as side chains and can also be very long groups of repeating structures. Branching polymers can be further categorized by how they branch off from the main chain. Polymers with many branches are known as dendrimers, and these molecules can form a webbing when cooled. This can make the polymer strong in the ideal temperature range. Such branched polymer chains can be modeled in terms of so-called quantum graphs, which are the set of nanoscale bonds connected at the vertices. The connection rule is called topology of a graph. Modeling of wave dynamics in branched conducting polymers require developing of effective methods allowing to take into account transition of the waves from one to another branches via the branching points. One of such approaches is based on the use of metric graphs as the models of the branched polymers. Within such approach, exciton dynamics can be modeled in terms of the Schrodinger equation on metric graphs.

We use solve the problem of exciton dynamics and charge separation (via splitting of exciton into electron and hole) by modeling the whole system in terms of quantum graph. The main problem we studied is splitting of exciton from transmission from one branch to another one. Charge separation probability is explicitly calculated.

Equilibrium colloidal gels under shear

José Ruiz-Franco[1], Nicoletta Gnan[2], Emanuela Zaccarelli[1,3]
[1]Dip. Di Fisica, Sapienza-Università di Roma, Roma, Italy. [2]CNR Institute of Complex Systems, Uos Sapienza, Rome, Italy. [3]CNR Institute of Complex Systems, Uos Sapienza, Roma, Italy

Soft matter systems have the intriguing property of forming a variety of different arrested states such as gels, repulsive or attractive glasses depending on the interaction potential and on the particle concentration. All of these arrested states are known to exhibit unique features when they are subjected to oscillatory or steady shear. However, understanding and controlling their dynamical response still

represent an open challenge for soft matter scientists. While several investigations have focused their attention on depletion-induced gels, at the moment there are no rheological studies on equilibrium gels obtained from the competition of short-range attraction and long-range repulsion interactions. It is then legitimate to ask whether there are universal features in the rheology of colloidal gelation or if there are aspects that depend on the specific colloid-colloid interactions. During the talk I will address this question by means of non-equilibrium molecular dynamics (NEMD) simulations of an equilibrium gel obtained *via* the competition of attraction and long-range repulsion under steady shear. By varying the Péclet number (Pe), I will show the effects of the shear flow on the structure, highlighting the onset of a crystallization transition for a given range of Pe. Furthermore, I will show the stress-strain relationship in comparison to different types of gels. In addition, I will present the limitations of the computational tools used so far and the possible advances that would allow to obtain a more realistic physical response.

Materials 9

Conference Center, Ballroom B

Fractal dimension of percolating interface in the spatial evolutionary games

Lev Shchur
Science Center oin Chernogolovka, Chernogolovka, Russian Federation

We investigate critical properties of a spatial evolutionary game based on the Prisoner's Dilemma. Simulations demonstrate a jump in the component densities accompanied by drastic changes in average sizes of the component clusters. Steady-state percolating clusters have dimension two. We measure properties of the percolating interface between clusters. Behaviour of the percolation interface is well known in statistical physics. In the case of the first-order phase transition the cluster boundary have dimension one. In the case of the second-order phase transition the cluster boundary have dimension between one and two. In our case neither situation was found. Contrary to both cases, our simulations are consistent with the fractal dimension of the cluster boundary being equal to 2.

Asymptotic-Preserving Simulation Methods for Non-Equilibrium Radiation Diffusion Problem

Xia Cui, Guang-Wei Yuan, Zhi-Jun Shen
Institute of Applied Physics and Computational Mathematics, Beijing, China

Studies on asymptotic-preserving numerical methods are very important for simulating complicated multi-physics with high efficiency and high fidelity. We extend the research in [D. A. Knoll, et al., J. Comput. Phys., 226 (2007) 1332-1347] on asymptotic-preserving temporally discrete methods for non-equilibrium radiation diffusion problem, and study the asymptotic-preserving spatially and fully discrete methods for non-equilibrium radiation diffusion problem in plane and curve geometry (spherical and cylindrical symmetric geometry). The research is based on two-temperature models with Larsen's flux-limited diffusion operators. Finite volume spatially discrete schemes are developed to circumvent the singularity at the origin and the polar axis and assure local conservation. Asymmetric second order accurate spatial approximation is utilized instead of the traditional first order one for boundary flux-limiters to consummate the schemes with higher order global consistency errors. The harmonic average approach in spherical geometry is analyzed, and its second order accuracy is demonstrated. Truncation errors for various discrete diffusion operators are derived. By formal analysis, we prove these schemes and their corresponding fully discrete schemes with implicitly balanced and linearly implicit time evolutions have first order asymptotic-preserving properties. By designing associated manufactured solutions and reference solutions, we verify the desired performance of the fully discrete schemes with numerical tests, which illustrates quantitatively they are first order asymptotic-preserving and basically second order accurate, hence competent for simulations of both equilibrium and non-equilibrium radiation diffusion problems.

Hole Doping of the Weak Itinerant Antiferromagnet TiAu

Milena Matthew, Wen Fong Goh, **Warren E. Pickett**
UC Davis, Davis, USA

The discovery of weak antiferromagnetism (wAFM) in metallic TiAu by Morosan's group has raised ques-

tions. Why is it magnetic, when neither Ti nor Au are magnetic metals? What determines the size of the ground state ordered moment, why is it commensurate, when most metallic AFMs are incommensurate. While we have made progress in answering these questions, new ones arise. Sc substitution for Ti (hole doping, $Ti_{1-x}Sc_xAu$) further weakens the magnetism and leads to the vanishing of magnetic order at the quantum critical point (QCP) x_c=0.12. Is the moment vanishing or just long-range order? We report computational study from two directions. First, the effects of disorder are minimized by using (i) the virtual crystal approximation (an average Ti-Sc atom) and (ii) the coherent potential approximation, in which electrons scattering off Ti and Sc atoms is approximated by scattering off an average site with a "coherent potential": an imaginary part describing disorder and a real-valued part. Second, we study supercells with a fraction x of Ti replaced by Sc (x=j/16 with several integer values of j). From the first two methods, we learn that xc is overestimated as might have been guessed from previous experience and the fact that spin fluctuations are ignored. From the real space method, we find, unexpectedly, that magnetism on the Ti atom persists well into the Ti-poor regime of this alloy system. The current picture of this system will be provided based on these results, compared to the experimental data.

New insight for hydrogen storage in the magnesium nickel and magnesium copper systems

Adlane Sayede, Gauthier Lefevre
UCCS - UMR CNRS 818, 1Université d'Artois, Faculté des Sciences Jean Perrin, Lens, France

In this work, efforts have been devoted to the theoretical investigation of binary systems with pressure consideration. An efficient predicition of stable alloys under pressure for magnesium-based system was performed at ab initio level. The effect of pressure change radically the minimal energy compositions and various rich-Mg coumpounds were found. Results are in agreement with recent exploration and new synthesis methods (1, 2). For intersting alloys, a careful investigation of potential hydrides has been performed, and electronic properties denote interesting informations on hydrogen atom behaviour in magnesium-based alloys. Results are giving attractive insights on identifying destabilized metal hydrides and encouraging the use of similar work to design hydride systems.

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Structure, Electronic, Vibrational Properties of Stanane and its Application as a Potential Gas Sensor

Vipin Kumar, Debesh R. Roy
Sardar Vallabhbhai National Institute of Technology, Surat, India

The charge transfer of toxic gas molecules (NO_2, SO_2, NH_3 and CO_2) on hexagonal chair type hydrogenated stanene has been studied in detail using density functional theory (DFT) based on an ab-initio

technique. The most stable configuration, electronic properties, adsorption energies and charge transfer of these gases on stanane are systematically discussed. The band gap of the pure stanane is noticed to be change 0.52 eV after interaction with gases. Moreover, the changes in the energy band gap and charge density is observed upon adsorption of NO_2, SO_2, NH_3 and CO_2 on p-type stanane based material. The results shows that the selectivity of hydrogenated stanene based gas sensors is very important to enhance their sensitivity. It is found that all the gas molecules act as charge donors in which NO_2 gas shows maximum adsorption their on the stanane surface along with maximum charge transfer. The nontrivial affectability and selectivity of stanane demonstrate that it has a potential application in the field of gas sensors and superior impetuses.

First principles study electronic properties of (110) surface GaAs/GaN nanowires

Chaib Youness[1], Benmokhtar Said[1], Moutaabbid Mohamed[1], Hoggan Phillip[2], Robert-Goumet Christinne[2]
[1]University of Casablanca, Laboratory of Chemistry and Physics of Materials LCPM, Faculty of Sciences, Department of Chemistry, Casablanca, Morocco. [2]Institute Pascal, UMR 6602 CNRS, University Blaise Pascal, Clermont-Ferrand, France

GaAs one of III-V compound semiconductor nanowires that exhibit direct band gap has attracted much attention of researchers due its potential application in the field of optoelectronic and microelectronic devices like photovoltaic cells, photo detectors, modulators, filters, integrated circuits and light emitting diodes [1,2], it has been widely studied both experimentally and theoretically, a fundamental understanding of its physical properties is still in demand of this novel material. During the manufacture of its nanowires, their surfaces present anomalies which bound to Ga-free broken bonds which are easily interacted with the environment and they oxidize for remedy this problem. We passivated these surfaces by the nitrogen for saturating their surfaces.

Motivated by the available literature on GaAs according to the crystalline plane (110), we carried out calculations for structural and electronic properties of GaAs in its stable zinc-blende phase using full potential linearized augmented plane wave method (FP-LPAW) designed within DFT. After that, we will passivate these nanowires by the nitrogen; we study the nutrient effect on their physical properties (GaAs / GaN) by keeping the same theoretical model used previously from a similar study that has been carried out on plane surfaces of GaAs showed that nitridation phenomena leads to the deposition of a thin layer of GaN and confers passivated to the solid [3].

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Discontinuous transition in a random growth lattice filling model of percolation

Sitangshu Bikas Santra, Bappaditya Roy
Indian Institute of Technology Guwahati, Guwahati, India

A random growth lattice filling model of percolation with touch and stop growth rule is studied numerically on a two dimensional square lattice. Nucleation centers are continuously added one at a time

to the empty lattice sites and clusters are grown from these nucleation centers with a growth probability g. For a given g, the system passes through a critical point during the growth process where a transition from a disconnected to connected phase occurs. The model is found to exhibit second order continuous percolation transitions as ordinary percolation for $g<0.5$ whereas for $g>0.8$ it exhibits weak first order discontinuous percolation transitions. The discontinuous transitions are characterized by compact spanning cluster, lattice size independent fluctuation of the order parameter per lattice, departure from power law scaling in the cluster size distribution and weak bimodal distribution of the order parameter. The nature of transitions are further confirmed by studying Binder cumulant. Instead of a sharp tricritical point, a tricritical region is found to occur for $0.5<g<0.8$ within which the values of the critical exponents change continuously till the crossover from continuous to discontinuous transition is completed.

Quantum Many-body 4

Conference Center, Ballroom C

Near-edge Absorption of HfO_2: Effect of Excitons

Xiao Zhang, Andre Schleife
University of Illinois at Urbana-Champaign, Urbana, USA

HfO_2 is a wide-gap dielectric material with high thermal stability and has applications in optical and protective coatings. It has been observed that the optical absorption spectrum of HfO_2 exhibits a shoulder-like feature near the absorption edge. This near band-edge behavior needs to be understood fully for device design, since it is a possible reason of the $\sim$ 0.4 eV lower band gap reported for crystalline HfO_2 compared to amorphous HfO_2. Several mechanisms including indirect band gap, defects, and self-trapped excitons are proposed to explain this feature. However, no solid conclusion has been drawn yet due to the complicated morphology in experiments, and the lack of accurate theoretical studies. In order to provide evidence of which mechanism dominates this feature, we investigated the optical absorption by performing first-principles calculations using both the independent particle approach and the Bethe-Salpeter equation (BSE) approach for monoclinic HfO_2. The BSE approach takes the screened electron-hole interaction into consideration and allows accurate predictions of optical spectra. We found that the shoulder-like feature becomes stronger as the electron-hole interactions, i.e. excitonic effects, become stronger and thus, conclude that excitonic effects are crucially affecting this feature. With further calculations using different screening parameters of the electron-hole interactions, we found that lattice screening is very important and needs to be taken into consideration to obtain accurate estimation of the optical spectrum of HfO_2.

Combining many-body perturbation theory with dynamical mean-field theory

Li Huang
China Academy of Engineering Physics, Mianyang, China

In the framework of the single-site dynamical mean-field theory, the momentum dependence of the electronic self-energy function is completely ignored. This approximation might not be true for low dimensional strongly correlated systems. In order to tackle this problem, some extensions of dynamical mean-field theory have been developed in the last decade, such as dynamical cluster approximation, cluster dynamical mean-field theory, dynamical vertex approximation, and dual fermion approach. Though these methods can recover the momentum dependence of self-energy function, the calculations are very heavy and tedious. Here, we propose an alternative approach with low computational cost, namely the combination of many-body perturbation theory and dynamical mean-field theory. In this approach, the non-local part of self-energy function is generated by the many-body perturbation theory, such as second-order perturbation theory, T-matrix approximation, GW approximation, and fluctuation-exchange approximation, while the local part is taken from the dynamical mean-field theory. We benchmark this approach in the 2D and 3D Hubbard models. We find that the calculated self-energy functions are in accord with those obtained by using the dynamical cluster approximation. Finally, we apply this new approach to study the electronic structures of strongly correlated metal $SrVO_3$. The calculated band structures successfully reproduce the main features as observed in the ARPES experiments.

The role of coupling constant in an inhomogeneous two-lane exclusion process model

Isha Dhiman
Thapar Institute of Engineering and Technology, Patiala, India

Nature presents plentiful examples of systems driven far away from equilibrium. In contrast to the systems in equilibrium, we do not have any general analytical framework which describes non-equilibrium systems in a unified manner. The most important property of a non-equilibrium system is the existence of non-zero particle current in its steady-state. In a driven lattice gas model (DLG), particles interact with their nearest neighbors and hop in a preferred direction. The asymmetric simple exclusion process (ASEP) is a specific example of DLG and is considered to be the simplest stochastic model for transport phenomena in which particles move along the lattice obeying hard-core exclusion principle with certain pre-assigned rules.

In particular, the real world situtations such as existence of a bottleneck in the flow, can be modeled using inhomogeneous ASEPs. This study is devoted to explore a two-lane system in the presence of a static bottleneck in one of the two lanes. The coupling constant C, which signifies the ratio of lane-changing rates, is introduced and the steady-state dynamics of the system are analyzed for different values of C. The stationary phase diagrams and various non-equilibrium phase transitions have been characterized in terms of C. It has been found that the coupling constant plays an influential role in the dynamics of the inhomogeneous system. The shock dynamics have also been investigated. We have also validated the results with extensively performed Monte Carlo simulations. Our theoretical arguments are in good agreement with Monte Carlo simulation results.

Two-dimensional solitary wave solution to the quadratic-cubic nonlinear Schrodinger equation

Sarun Phibanchon[1], Yuttakarn Rattanachai[2]
[1]Faculty of Education, Burapha University, Chonburi, Thailand. [2]Department of Applied Physics, Rajamangala University of Technology Isan, Nakorn Ratchasima, Thailand

The Madelung fluid transformation is applied to find the link between the modified Korteweg-de Vries and and the quadratic-cubic nonlinear Schrdinger equation. The two-dimensional solitary wave solution of the quadratic-cubic nonlinear Schrdinger equation will be determined by the Petviashvili method. This solution will be used for the initial condition for the time evolution to study the stability analysis. The spectral method is applied for the time evolution.

Adomian Decomposition Method for the dark solitons solution to the modified Korteweg-de Vries equation

Songvudhi Chimchinda[1], Sarun Phibanchon[2]
[1]Physics Department, Burapha University, Chonburi, Thailand. [2]Faculty of Education, Burapha University, Chonburi, Thailand

The Adomian decomposition method (ADM), is the one of the semi-analytical method, will be applied to study the time evolution of the dark soliton solution to the modified Korteweg-de Vries equation. We also provide the conservation laws to verify the dark solution obtained from this method. The ADM gives a good result for the approximation solution of the weakly nonlinear wave equation.

Charged Defects in Two-dimensional Materials from Many Body Perturbation Theory

Yuan Ping[1], Ravishankar Sundararaman[2], Dario Rocca[3], Feng Wu[1]
[1]*University of California, Santa Cruz, Santa Cruz, USA.* [2]*Rensselaer Polytechnic Institute, Troy, USA.* [3]*Université de Lorraine, Nancy, France*

Recently, defects in 2D materials such as ultrathin h-BN have been found to be promising single-photon emitters with polarized and ultrabright single-photon emission at room temperature. This opens up possibilities for emerging applications in nanophotonics and quantum information, with potentially much better scalability than the long-studied nitrogen vacancy (NV^-) in diamond. Despite of promising properties experimentally demonstrated so far, first-principles prediction of accurate defect properties in 2D materials remains challenging, mainly because of the highly anisotropic dielectric screening in 2D materials and strong many body interactions including electron-hole, electron-phonon and defect-exciton interactions, which could not be treated by standard density functional theory codes.

The talk will discuss how we solved the numerical convergence issues for charged defect properties in 2D materials at both the DFT and MBPT levels, and how we will tackle the complex many body interactions for the excited state properties of defective 2D materials and heterojunctions. In particular, we resolved the long-standing issues of dealing with charged defects in 2D materials from first-principles, which necessitates proper treatment of electrostatic potentials of charges near a 2D plane and of the screened Coulomb interaction in the MBPT.[1] With our methods, we will design promising quantum defects that have deep defect levels, high spin states, bright optical excitations between defect states, long excited state lifetime and high photoluminescence efficiency. [1]W. Feng, A. Galatas, R. Sundararaman, D. Rocca and Y. Ping, *Physical Review Materials (Rapid Communication)*, 1, 071001(R) (2017)