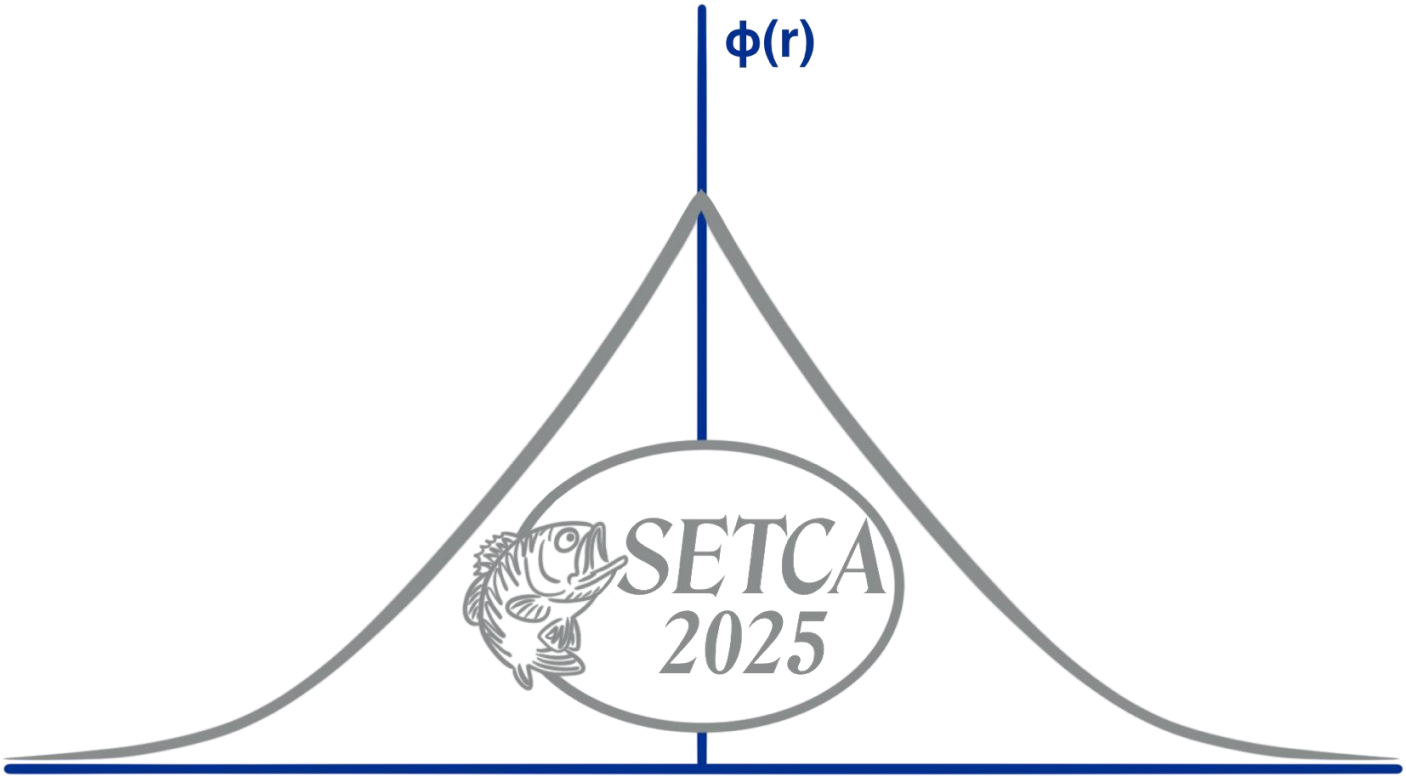

The 53rd Annual Meeting of the Southeastern Theoretical Chemistry Association

May 8 – 10, 2025

University of Memphis
Memphis, TN

Contents

Timetable

Thursday, May 8th

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5:00–6:00 pm	**Check-in**
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IT: Invited Talk, CT: Contributed Talk

Friday Morning, May 9th (Presider: Dr. Dominique Wappert)

8:30–9:00 am	**Check-in**		
9:00–9:15 am	**Opening remarks**		
9:15–9:40 am	IT1	**Daniel Crawford** Virginia Tech	Advanced Quantum Chemical Methods for Chiroptical Spectroscopy
9:40–10:05 am	IT2	**Devin Matthews** Southern Methodist University	Tensor Factorization Techniques for Coupled Cluster Methods
10:05–10:30 am	IT3	**Eugene DePrince** Florida State University	Lower Bounds in Quantum Chemistry
10:30–10:50 am	**Coffee Break**		
10:50–11:15 am	IT4	**Francesco Evangelista** Emory University	Mutual Correlation
11:15–11:40 am	IT5	**Jay Foley** University of North Carolina at Charlotte	*Ab initio* Cavity Quantum Electrodynamics
11:40–12:00 pm	CT1	**Shengli Zou** University of Central Florida	Revealing the Collapse Mechanism of Photons via a Nanoparticle Dimer or Multiple Emitters Near a Metallic Nanoparticle
12:00–2:00 pm	**Poster Session II & Lunch**		

Friday Afternoon, May 9th (Presider: Dr. Megan Simons)

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3:15–3:35 pm	**Coffee Break**		
3:35–4:00 pm	IT9	**Edward Valeev** Virginia Tech	Beyond atomic orbitals and plane waves: multiwavelet representations for converged correlated all-electron simulation of molecules and solids
4:00–4:25 pm	IT10	**Małgorzata Makoś** The University of Alabama	Adaptive-Learning Reaction Pathways Search
4:25–4:50 pm	IT11	**Konrad Patkowski** Auburn University	Symmetry-adapted perturbation theory, but not for two molecules
4:50–5:10 pm	CT2	**James Baird** University of Alabama in Huntsville	Electrostatic Energy of a Dipolar Ion in an Electrolyte Solution
6:00–8:00 pm	**Dinner Reception**		

Saturday Morning, May 10th (Presider: Dr. Sarah Pak)

9:00–9:25 am	IT12	**Elisa Pieri** University of North Carolina at Chapel Hill	Modeling the titration of biological chromophores in complex environments
9:25–9:45 am	CT3	**Greg Tschumper** Missouri University of Science and Technology	Concerted Proton Transfer in Small Cyclic Hydrogen Bonded Clusters
9:45–10:05 am	CT4	**Ilias Magoulas** Emory University	Clifford Transformations for Fermionic Quantum Systems: From Paulis to Majoranas to Fermions
10:05–10:25 am	CT5	**Ryan Fortenberry** University of Mississippi	PAHsing to Compute IR Spectra
10:25–10:45 am	**Coffee Break**		
10:45–11:10 am	IT13	**Lee Thompson** University of Louisville	Beyond Orthogonality: Nonadiabatic Chemistry through a Nonorthogonal Lens
11:10–11:35 am	IT14	**Justin Talbot** Clemson University	Bridging the gaps in quantum chemistry: Integrating electronic structure and molecular dynamics
11:35–12:00 pm	IT15	**Samer Gozem** Georgia State University	Revisiting Oscillator Strength Calculations for Solvated Molecules
12:00–12:30 pm	**Concluding remarks and business meeting**		

List of Abstracts – Talks

Friday Morning, May 9th (Presider: Dr. Dominique Wappert)

Advanced Quantum Chemical Methods for Chiroptical Spectroscopy

T. Daniel Crawford

IT1

Virginia Tech

The determination of the “handedness” of chiral compounds remains a fascinating and critical challenge in which theory and computation play a vital role. In the effort to assign the absolute stereochemical configurations of chiral isolates, quantum chemical models have the potential to provide experimentalists with robust predictions of the requisite spectroscopic signatures, such as specific rotation, circular dichroism rotatory strengths, Raman scattering circular intensity differences, and more. However, such properties are among the most challenging to simulate because of their delicate dependence on a variety of intrinsic and extrinsic factors. In this lecture, I will I discuss recent efforts toward the goal of developing reliable theoretical predictions of chiroptical properties, including the exploration of reduced-scaling techniques, new wave-function-based methods for vibrational circular dichroism spectra, and explicitly time-dependent quantum dynamics.

Tensor Factorization Techniques for Coupled Cluster Methods

Devin A. Matthews

IT2

Southern Methodist University

Coupled cluster (CC) methods are notorious for extreme computational cost via high polynomial scaling, although they provide a very rapid and reliable convergence to the full CI limit for most molecular systems. Thus, scaling reduction is an important effort which promises to extend the reach of CC accuracy to larger and more varied molecules. In this talk, I will explore both the least-squares tensor hypercontraction (LS-THC) and rank-reduced/singular valued decomposed (RR/SVD) families of approximations as applied to CC. These techniques reduce the scaling of CC, for example LS-THC-CCSD reduced from $O(N^6)$ to $O(N^4)$, while RR-CCSD(T) and RR-CCSDT are reduced from $O(N^7)$ and $O(N^8)$, respectively, to $O(N^6)$. However, many open questions remain on how to best balance accuracy and computational cost, how to extend to more types of systems, techniques, and applications, among others. In particular, the extension of LS-THC to open-shell systems, a more accurate LS-THC representation of the doubles amplitudes, and the application of RR-CCSD(T) to problems of thermochemical relevance will be covered in this talk.

Lower Bounds in Quantum Chemistry

Eugene DePrince

IT3

Florida State University

Any electronic Hamiltonian can be decomposed into a sum of squares (SOS) of products of fermionic creation and annihilation operators plus a constant shift. The constant shift is a lower- bound to the ground-state energy of the Hamiltonian, and a tighter lower-bound can be obtained as the pool of fermionic operators becomes more complete. The SOS decomposition problem is a complement to a more well-known approach in quantum chemistry based on the variational optimization of the two-electron reduced density matrix (2RDM). In this approach, the 2RDM is optimized subject to a set of ensemble N-representability conditions, and, as the set of conditions becomes more complete, the trace of the 2RDM against the Hamiltonian approaches the full configuration interaction energy from below. In this talk, I will discuss the similarities and differences between the SOS and variational 2RDM approaches.

Mutual Correlation

Francesco Evangelista

IT4

Emory University

Understanding and quantifying electron correlation remains a critical challenge in electronic structure theory and condensed matter physics, and is related to the problem of establishing the complexity of a quantum state from the perspective of quantum information science. In this talk, I will introduce a new correlation metric, termed mutual correlation, derived from the Frobenius norm squared of the two-particle reduced density matrix cumulant. Mutual correlation uniquely captures nonadditive interactions between subsystems and provides an intuitive, computationally efficient alternative to entropy-based measures like orbital mutual information. Applications to molecular and model systems and small molecules will illustrate how mutual correlation effectively identifies strong correlations, facilitates active space selection, and aids in interpreting electronic structure calculations. This metric's simplicity, numerical stability, and general applicability make it an attractive tool for theoretical exploration and practical computations in quantum chemistry.

Ab initio Cavity Quantum Electrodynamics

Jay Foley IT5

University of North Carolina at Charlotte

Polariton chemistry exploits the strong interaction between quantized excitations in molecules and quantized photon states in optical cavities to affect chemical reactivity. Molecular polaritons have been experimentally realized by the coupling of electronic, vibrational, and rovibrational transitions to photon modes, which has spurred tremendous theoretical effort to model and explain how polariton formation can influence chemistry. I will present recent work in my group aimed at making the accurate computational modeling of molecular polaritons and molecules under strong light-matter coupling routine. In particular, I will describe a class of approaches called *ab initio* cavity quantum electrodynamics that treat molecular electronic degrees of freedom and photon degrees of freedom on equal quantum mechanical footing, and can provide atomistic detail into the structure and reactivity of molecules under strong light-matter coupling. I will also highlight some pedagogical developments that we have developed to introduce students to computational molecular science tools within the context of strong light-matter coupling.

Revealing the Collapse Mechanism of Photons via a Nanoparticle Dimer or Multiple Emitters Near a Metallic Nanoparticle

Shengli Zou CT1

University of Central Florida

Photons are among the most commonly observed yet most mysterious forms of matter. One of their most fascinating properties is wave-particle duality. When photons interact with matter, the interaction causes the collapse of the photon's wavefunction, revealing its particle properties. However, the precise mechanisms of when and how this wavefunction collapse occurs remain unclear. In our work, we use a nanoparticle dimer to simulate the conventional double-slit experiment, with the goal of uncovering the collapse mechanism of photons during interactions with nanoparticles. Additionally, we designed experiments involving multiple emitters near metallic nanoparticles. Depending on the collapse mechanism of the photons, these two experimental setups are expected to yield completely different results. We anticipate that experimental verification of the theoretically designed experiments will shed light on the intrinsic properties of light-matter interactions. Our findings could not only enhance our fundamental understanding of photon wave-particle duality but also have significant implications for quantum communication, where the collapse of quantum states is of particular interest.

Friday Afternoon, May 9th (Presider: Dr. Megan Simons)

Real-time simulations of ultrafast electron relaxation dynamics

Joshua Kretchmer

IT6

Georgia Tech

The ionization of an inner-shell electron in weakly bound systems can initiate a multitude of competing electronic relaxation pathways that occur on the ultrafast timescale. An electron relaxes to fill the hole, which can simultaneously ionize a low-energy secondary electron. However, the location of the electron that relaxes and the secondary ionized electron can originate from either the original molecule or a neighboring molecule. The relaxation can also compete with electron, hole, and even proton transfer. In this talk, I will discuss our recent work developing a new methodology based on real-time DFT to simulate the explicit dynamics of this complex array of processes. We can account for the secondary ionization event by combining a non-Hermitian form of real-time DFT with a complex absorbing potential. We additionally introduce coupled electron-nuclear dynamics through Ehrenfest dynamics, which enables an in-depth investigation of the fragmentation pathways in the water dimer following an inner-valence ionization event.

Quantum Dynamics with Gaussian Bases: Theme and Variations

Sophya Garashchuk

IT7

University of South Carolina

Importance of the quantum-mechanical effects associated with the nuclei is gaining recognition in chemistry and physics, as researchers manipulate matter, light, electric and magnetic fields at the atomistic level for advanced materials applications. For example, the isotope dependence of the proton conductance in low-dimensional boron nitrides, and of the crystallinity of poly(3-hexylthiophene) is attributed, in part, to the nuclear quantum effects. The development of a general dynamics approach, incorporating the nuclear quantum effects and scalable to large molecular systems, remains an outstanding theoretical challenge because of the exponential scaling of computational costs with the system size. We will discuss application or the time-dependent variational principle to the trajectory-driven bases, and describe exact and approximate dynamics, inspired by the quantum trajectory formulation of the Schrödinger equation [1,2]. The significance of the quantum behavior of the nuclei will be illustrated on the case study of the Kinetic Isotope Effect in Cytochrome P450 Decarboxylase OleT [3], attributed in part to quantum tunneling.

References

[1] M. Dutra, S. Wickramasinghe, and S. Garashchuk. Quantum Dynamics with the Quantum Trajectory-Guided Adaptable Gaussian Bases. Journal of Chemical Theory and Computation 16, 18-34 (2020). DOI: 10.1021/acs.jctc.9b00844

[2] S. Garashchuk, and F. Großmann. Assessing the Accuracy of Quantum Dynamics Performed in the Time-Dependent Basis Representation. J Phys Chem A 128, 8265-8278 (2024). DOI: 10.1021/acs.jpca.4c03657.

[3] M. Dutra, et al. Experimental and Theoretical Examination of the Kinetic Isotope Effect in Cytochrome P450 Decarboxylase OleT. J. Phys. Chem. B 126 (19), 3493-3504 (2022). DOI: 10.1021/acs.jpcb.1c10280.

TBA

Nicholas Mayhall

IT8

Virginia Tech

Beyond atomic orbitals and plane waves: multiwavelet representations for converged correlated all-electron simulation of molecules and solids

Edward Valeev

IT9

Virginia Tech

The dominant numerical representations for the electronic structure simulation of periodic solids, namely, plane waves augmented with pseudopotentials and the atomic orbitals, are inadequate for confident control of numerical error, especially for all-electron simulation. To address their shortcomings we extended the adaptive multiwavelet numerical technology to the treatment of periodic solids using the mean-field methods (Hartree–Fock and semilocal and generalized Kohn-Sham density functional theory). To address the unphysical periodicity of reduced density matrices due to the finite quadrature over the first Brillouin zone it is mandatory to use a modified Poisson kernel that smoothly restricts its range in a manner similar to the approach used for the optimal plane-wave evaluation of the exact exchange operator.[1] The use of the modified kernel yields the exponential convergence to the thermodynamic limit for mean-field models of non-metals while enjoying the optimal rate of convergence of the numerical error; this approach also eliminates the well-known divergence of the exact exchange energy.[2] The current implementation is Γ-point only, but the efficiency will be soon improved further by explicit utilization of translational (k-point) symmetry. The periodic extension of the MW technology has been incorporated into the universal correlated orbital solver,[3] positioning it for the use with correlated electronic structure simulation of periodic solids.

References

1. R. Sundararaman, and T. A. Arias, Phys. Rev. B 87, 165122 (2013).
2. C. Pisani, R. Dovesi, and C. Roetti. Hartree-Fock Ab Initio Treatment of Crystalline Systems (1988).
3. E. F. Valeev, R. J. Harrison, A. A. Holmes, C, C. Peterson, and D. A. Penchoff, J. Chem. Theor. Comput. 19 (20), 7230-7241 (2023).

Adaptive-Learning Reaction Pathways Search

Małgorzata Z. Makoś

IT10

The University of Alabama

The search for reaction pathways is a crucial aspect of chemistry, with numerous applications in drug design, materials science, and catalysis. It involves exploring the energy landscape of complex chemical reactions to identify the reactants, transition states, and products. However, this task is incredibly challenging, as it requires navigating a vast potential energy surface with multiple possible outcomes.

Here, we propose an adaptive learning global optimizer combined with a machine learning algorithm to explore the potential energy surface and identify the reaction pathways. The recently developed global optimization algorithm allows for the determination of low-energy minima for large systems and has an interface to numerous quantum chemistry and molecular dynamics software. Generative adversarial networks have been successfully used for the prediction of the transition states between a given set of reactants and products. Here, we combine the two computational schemes to connect a large set of possible reactants, transition states, and products, together with calculated energies at the DFT level.

Our approach has been successfully used in identifying the mechanisms of various chemical reactions, including those involving surface reactions. This approach aid in the discovery of new reactions, optimization of existing reactions, the prediction of reaction outcomes, and extraction of generalized system descriptors. Moreover, it can facilitate the development of more efficient and sustainable chemical processes, contributing to the advancement of the chemical industry.

Symmetry-adapted perturbation theory, but not for two molecules

Konrad Patkowski

IT11

Auburn University

In its most standard variants, symmetry-adapted perturbation theory (SAPT) is a popular method to compute an interaction energy between two molecules in terms of physical components such as the electrostatic, induction, dispersion, and exchange energies. However, the underlying physics of the interaction is the same for any number of molecules, and it is useful to construct and refine SAPT-based approaches to either one molecule (with noncovalently interacting fragments) or three or more molecules. In the first case, an intramolecular ISAPT variant has been developed to compute interaction energy components between fragments A and B covalently connected through a linker C. However, the results are sensitive to how the interfragment boundaries are treated, and our group proposed an ISAPT variant where unphysical dipole moments at those boundaries are substantially reduced. Such an ISAPT approach gives reasonable results for all A-B-C fragmentation patterns and has been used to compute and interpret intramolecular forces in pentanediols, linear and branched alkanes, open and closed conformations of molecular balances, and substituted cis- and trans- azobenzenes. Moreover, our group is working on extending ISAPT to describe the entire nonbonded energy in a molecule (as opposed to its A-B component for specific fragments), replacing molecular fragmentation by a range separation of the interaction potential. We showed that the noncovalent interaction can be well reproduced by limiting this potential to its long-range part. In the case of three molecules, leading-order SAPT contributions to the nonadditive interaction energy have been developed a long time ago. In addition, the nonadditive induction effects can be iteratively included for any number of molecules within the extended SAPT (XSAPT) approach. We recently compared the performance of several two- and three-body SAPT variants with accurate supermolecular reference data for a set of 20 trimer structures including up to 3 different molecules, and are now developing a larger benchmark set that focuses on halogen-bonded pairs interacting with a third molecule. We show that while in principle SAPT can account for all important nonadditive effects in molecular trimers, the three-body dispersion contribution is typically overestimated and should be studied further, while also considering alternatives such as the many-body dispersion (MBD) approach.

Electrostatic Energy of a Dipolar Ion in an Electrolyte Solution

James K. Baird

CT2

University of Alabama in Huntsville

In aqueous solution, amino acids exist as dipolar ions, as do proteins when the solution pH = pI, where pI is the isoelectric point of the protein molecule. When the solution contains a supporting electrolyte, it is observed that the solubility of a dipolar solute depends upon the electrolyte concentration. Following the lead of Bruno Linder [1], the founder of SETCA, and a champion of the Onsager electrostatic reaction field theory of dielectrics [2], we apply the theory to calculate the electrostatic potential of the dipolar ion in solution. We solve Laplace's equation for electrostatic potential associated with the dipole and the Debye – Huckel equation for the electrostatic potential associated with the surrounding electrolyte. Both partial differential equations admit exact solutions, which when combined permit a closed form evaluation of the electrostatic energy of the dipolar ion as it depends upon temperature and ionic strength. The resulting energy formula also applies in the case of plasma screening of a dipole in the gas phase. Because of the low dielectric permittivity of vacuum (unity), as compared to the high permittivity of water (eighty), the predictions in the case of the gaseous plasma are quite different from the predictions that apply in the case of the aqueous solution.

References

[1] B. Linder, Adv. Chem. Phys. 12, 225 – 282 (1967).
[2] L. Onsager, J. Am. Chem. Soc. 58, 1486 – 1493 (1936).

Saturday Morning, May 10th (Presider: Dr. Sarah Pak)

Modeling the titration of biological chromophores in complex environments

Elisa Pieri

IT12

University of North Carolina at Chapel Hill

The pH significantly influences the light-driven activity of proteins by affecting electrostatic interactions and steric hindrance. These changes alter the protonation states of amino acids within the chromophore's binding pocket, leading to shifts in absorption and emission spectra and modifying the excited state dynamics. Notably, the protonation state of the chromophore itself has the most substantial impact. Biliverdin, with its elusive pKa values in water, serves as an intriguing case study. This polyprotic chromophore, prevalent in various protein families, often exhibits uncertain protonation states. Using extensive data from a customized constant pH molecular dynamics (CpHMD) implementation, we model the titration of biliverdin through a microstate approach. Furthermore, we investigate how the oligomerization of Sandercyanin influences biliverdin's pKa values and the subsequent effects on chromophore binding.

Concerted Proton Transfer in Small Cyclic Hydrogen Bonded Clusters

Greg Tschumper

CT3

Missouri University of Science and Technology

This work examines small cyclic hydrogen-bonded clusters composed of H_2O, HF and HCl as well as the corresponding transition states for concerted proton transfer. Benchmark results for the homogeneous systems have been used to calibrate less-demanding procedures that were subsequently employed to characterize the heterogeneous systems. Several heterogeneous trimers and tetramers have been identified with barriers for concerted proton transfer that are likely sufficiently low to enable the experimental detection of many-body tunneling in these systems via tunneling splittings in high-resolution gas-phase vibrational spectra.

Clifford Transformations for Fermionic Quantum Systems: From Paulis to Majoranas to Fermions

Ilias Magoulas and Francesco A. Evangelista

CT4

Emory University

Clifford gates and transformations, which map products of Pauli or Majorana operators onto similar products, are foundational in quantum computing, underpinning, among others, the stabilizer formalism, quantum error correction, magic state distillation, quantum communication, and qubit tapering. Moreover, circuits composed entirely of Clifford gates are classically simulatable, emphasizing their computational significance. In this work, we utilize the exact, closed-form unitary transformations of fermionic operators that we recently derived to extend the concept of Clifford transformations to fermionic operators. We demonstrate that fermionic Clifford transformations are generated by half-body and pair operators, thus providing a systematic framework for their characterization. We further illustrate the clear physical interpretation of these transformations, which give rise to particle-hole conjugations, spin-flip transformations, and swapping of spinorbital indices. Using the minimum-basis-set H_2 molecule as an illustrative example, we highlight the role of fermionic Clifford transformations in qubit tapering. Finally, by generalizing fermionic Clifford transformations, we establish connections with all known flavors of mean-field theories.

PAHsing to Compute IR Spectra

Ryan C. Fortenberry & Vincent J. Esposito

CT5

University of Mississippi

The spectral assignment of several CN-functionalized polycyclic aromatic hydrocarbons (CN-PAHs) is provided from quantum chemical computations in direct support of James Webb Space Telescope observations. As much as 20% of the carbon in the universe is believed to be tied up in polycyclic aromatic hydrocarbons (PAHs). While hints to their presence in space have been known for more than half a century, only recent detections of strongly dipolar, CN-functionalized PAHs have clearly shown that PAHs and PAH-like molecules are present in astronomical regions like the Taurus Molecular Cloud. Part of this lack of clear attribution has been due to a lack reference, experimental spectral data as well as the difficulty in characterizing the spectra of PAHs even when they're produced due to the largely blended spectral features that characterize PAHs as they aggregate even in the gas phase. As such, computation can treat one PAH or CN-PAH at a time and blend the spectra together from the bottom up. This work showcases that the region around the CN stretch in known CN-PAHs is relatively narrow and that other IR regions become much more complicated upon CN functionalization than in standard PAHs. It also highlights new developments in quantum chemical techniques that are necessary for such computations to be possible.

Beyond Orthogonality: Nonadiabatic Chemistry through a Nonorthogonal Lens

Lee M. Thompson

IT13

University of Louisville

Nonadiabatic processes underpin key phenomena in photochemistry, energy transfer, and catalysis. These processes are marked by strong interactions between electronic motion and a time-dependent external perturbation, such as light, electric fields, or nuclear motion, that induces coupling between the electronic eigenstates. Accurate computational modeling of such processes is essential but remains challenging due to significant orbital relaxation, multielectron excitations, and the need to capture multiple near-degenerate electronic states. To address these challenges, our group has focused on wavefunction theories that incorporate nonorthogonal determinant expansions to more effectively capture key components of the wavefunction. These methods exploit the flexibility of using configuration-specific orbitals, yielding compact, chemically intuitive representations of strongly correlated wavefunctions. In this work, I will describe how the nonorthogonal framework is being used for resolving challenges in modeling transition metal and lanthanide electronic structure, kinetics of energy transfer processes, and electron dynamics induced by low-kinetic energy photodetachment.

Bridging the gaps in quantum chemistry: Integrating electronic structure and molecular dynamics

Justin J. Talbot

IT14

Clemson University

Elucidating the role of nonadiabatic transitions in renewable energy catalysis, biological processes, and atmospheric chemistry remains a significant challenge for computational chemistry. Addressing this problem requires integrated electronic and vibrational structure models that can reliably describe excited-state potential energy surfaces and the couplings that drive population transfer between them. To this end, we have developed an approach that incorporates density functional theory—including the analytic evaluation of non-adiabatic couplings—with the symmetric quasi-classical Meyer-Miller model which treats the electronic and nuclear motions on an equal footing using classical mechanics. In this talk, I will discuss the strengths and limitations of this approach and illustrate, using small gas-phase molecules, how it can capture complex dynamics relevant to ultrafast spectroscopies and energy flow within molecules. I will also briefly highlight ongoing directions in my group, including efforts to model internal conversion pathways in realistic solar energy chromophores, develop improved models to calculate binding thermodynamics of adsorbed atoms and molecules, and interpret anomalous infrared signatures of reactive ions.

Revisiting Oscillator Strength Calculations for Solvated Molecules

Samer Gozem

IT15

Georgia State University

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P16	**Zihui Song; Jonathan S. Bersson ; Lee M. Thompson**	Revealing correlation mechanisms through nonorthogonal multiconfiguration self-consistent field calculations
P17	**Megan J. Mackintosh, Lee M. Thompson**	Beyond non-orthogonal wave functions: Recovering correlation energy via perturbation theory for applications in excited-state processes
P18	**Andrei Evdokimov, Valentina Nesterova, Marcelo Kuroda, Konstantin Klyukin, Evangelos Miliordos**	Ab initio design of new 2-dimensional electrides with hybrid electronic structures
P19	**Zijun Zhao, Shuhang Li, and Francesco A. Evangelista**	Multireference equation-of-motion formalism based on the driven similarity renormalization group: theoretical foundations and applications to ionized states
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Friday Session

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P4	**Stephen Ajagbe, Paulami Ghosh, Samer Gozem**	Tuning mechanisms for intersystem crossing in LOV2 vs LOV1 domains of Phototropins.
P5	**Paulami Ghosh, Stephen O. Ajagbe, Samer Gozem***	Multiple tuning mechanisms for intersystem crossing in LOV2 vs LOV1 domains of phototropins: All paths lead to the triplet state.

P6	**Sarah Elhajj, Jacopo D'Ascenzi, Samer Gozem**	APEC-F 2.0: Implementing Automated QM/MM Modeling for Flavoproteins for Fluorescent Protein Simulations and Redox Potential Calculations.
P7	**Mikhayla Clothier, Samhitha Venkat, Dariia Yehorova, Joshua S. Kretchmer**	Development of Spin-Generalized Real-Time Projected Density Matrix Embedding Theory
P8	**Alexandros Androutsopoulos and Evangelos Miliordos**	Insights Into the Electronic Structure of (Ti-CO2)- and (V-CO2)- Species
P9	**Chinmay Shrikhande, Nicholas Mayhall**	Selected CI for Lindbladian Superoperators: Avoiding the Cost of Full Diagonalization
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P11	**Chao Yin, James H. Thorpe, Devin A. Matthews**	Energy Pivoting in Least-Sqaures Tensor Hyper-Contraction
P12	**Sharon Ochieng and Konrad Patkowski**	Influence of three body effects on Halogen bonding
P13	**Daniel P. Devore and Devin A. Matthews**	Scaling Reduction in Open-Shell CCSD(T) through Tensor Decomposition
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P19	**Victor Suarez, Joshua Kretchmer**	Kinetically-constrained ring-polymer molecular dynamics for chemical reactions spanning the non-adiabatic to adiabatic regime
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P21	**Muhan Zhang, Ilias Magoulas, Francesco A. Evangelista**	Symmetry Projection on Quantum Computers: Shaping the Future of Hardware-Friendly Ansätze
P22	**Muhammed A. Dada and Daniel R. Nascimento**	Simulating resonant inelastic x-ray scattering of Ru model complexes using time-dependent density functional theory
P23	**Dillon T.A. Baker, Brinton King Eldridge, Yongmei Wang**	PolyCrit: An Online Database and Machine Learning Framework for Polymer Characterization by Polymer LCCC
P24	**Nicholas Corsello, Sergei Egorov**	Calculation of the Quantum Mechanical Effusion Rate via Miller's Method

P25	**Dr. Reza Hemmati and Dr. Benjamin Pritchard**	Implementation of the Gaussian electronic structure program into QCArchive, an open-source ecosystem for large-scale quantum chemistry computations
P26	**John P. Pederson, Jesse G. McDaniel**	Extending Generalized Hybrid Orbitals (GHO) to Model QM/MM Boundaries in Solid Surfaces
P27	**Jose P. Madriaga and Dr. Daniel Crawford**	Speeding Through the Highs and Lows of PNO-CC Response Methods
P28	**Arnab Bachhar, Nicholas Mayhall**	Exploring transition metal chemistry using tensor product selected configuration interaction method
P29	**Jinyi Zhang, HongjunLiu, De-en Jiang**	Li+ ion transport in high concentration electrolyte (HCE)
P30	**Matthew N. Ward, Daniel R. Nascimento**	Effect of Numerical Integration Grids in TD-DFT Core-Level Spectra Calculations
P31	**Sarah Pak, Muhammed Dada, Niranjan (Niri) Govind, and Daniel R. Nascimento**	Fast simulation of soft x-ray near-edge spectra using a relativistic state-interaction approach: Application to closed-shell transition metal complexes
P32	**Stephen H. Yuwono, Run R. Li, A. Eugene DePrince III**	Completely Renormalized Equation-of-Motion Coupled Cluster in the Exact Two-Component Relativistic Framework
P33	**Eugene DePrince**	The Exact Electron-Photon Exchange-Correlation Potential in Cavity Quantum Electrodynamics Density Functional Theory
P34	**P.D. Varuna S. Pathirage, Stephen H. Yuwono, A. Eugene DePrince III**	Implementation of Ionization-Potential and Electron-Attachment Time-Dependent Equation-of-Motion Coupled-Cluster with Koopman Initial States
P35	**Urvashi; Hossain Shadman; Xiaohua Huang ; Yongmei Wang**	Analysis of Integrin & CEACAM Expression in Breast Cancer Using GTEx and TCGA data
P36	**Jordan Hale, Mikhayla Clothier, Joshua S. Kretchmer**	Investigating Interlayer Charge Transport of 2D Hybrid Perovskites via Constrained Density Functional Theory
P37	**Tatyana Denton, Sophia Mohamed, Katherine Crutchfield, Lauren Roberts, Emma Wallace, Serena D. Stoddard, Shana V. Stoddard**	Advancing Homology Modeling: Strategies for Complex Multidomain Fibrous Proteins
P38	**David H. Magers**	Ring strain of cylopropane, cyclobutane, and small heterocycles revisited

List of Abstracts – Posters

Thursday Session

Characterization of Novel Actinide Fluoride Compounds Using Electronic Structure Methods

Jackson Maxwell*, *Kayleigh Barlow*, *David Dixon

P1

The University of Alabama

Understanding the properties of actinide compounds is important for nuclear energy production as well as for environmental remediation from the production of nuclear weapons and nuclear energy. There is substantial interest in the fundamental properties of actinide compounds due to the presence of 5f electrons. The geometries and electronic structures of early actinide fluorides, AnF_n (An=Ac, Th, Pa, U), where n is the normal maximum oxidation state for the actinide, were studied using advanced computational electronic structure methods. Novel structures were predicted for the actinide fluorides when they have an additional fluorine above the number needed for the highest oxidation or in the cation derived from the highest oxidation state normal fluoride. These novel structures are of the form $[AnF^{+}_{(n-1)}][F_2^-]$ and $[AnF^{2+}_{(n-2)}][F_2^-]$ respectively. Forming F_2^- complexes allows the actinides to maintain their oxidation state, making them the most stable structures. When $[AnF^{+}_{(n-1)}][F_2^-]$ loses an electron, the electron is taken from the F_2^- to form an $[AnF^{+}_{(n-1)}][F_2]$ complex, where F_2 is weakly bound.

Machine Learning for Thermochemistry of Transition Metal (II) Oxides from Electronic Structure Theory

Nickolas Joyner*, *Sarah Sprouse*, *Kathleen Butler*, *Elliot Kaye*, *Malgorzata Makos**, *David A. Dixon

P2

The University of Alabama

High accuracy predictions of the thermochemical and kinetic properties of large transition metal oxide nanoparticles are often limited due to the computational cost requirements associated with large systems. To overcome these obstacles, a novel machine learning method has been developed to enhance the accuracy of electronic structure methods. This machine learning algorithm increases the accuracy of thermochemical properties, such as the normalized clustering energy (NCE), calculated by density functional theory to correlated molecular orbital theory level. This is done using two distinct algorithms. The first algorithm predicts the thermochemical property of the transition metal oxide. The second algorithm generates a correction which is calculated by the difference between the property calculated at high and low level of theory. This correction is then applied to the prediction generated from the first algorithm. The two algorithms have been implemented to generate the initial thermochemical predictions. Kernel ridge regression, using the smooth overlap of atomic orbital as a molecular descriptor, is able to provide predictions that are within 0.566 kcal/mol of initial DFT calculated values. Other architectures such as a sequential neural network, have been tested and provide values that are within 2 kcal/mol of initial DFT values. These algorithms can predict NCEs of a wide range of transition metal oxides. The NCEs when plotted against the cluster size as n-1/3 can then be used to predict cohesive energies of metal oxides and subsequently heats of formation of bulk metal oxides. Further work is underway to build the correction algorithm. This work was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Division of Chemical Sciences.

Methane Activation by Single Metal Anions: A Combined Computational and Experimental Study

Joseph Olaniyan*, *Evangelos Miliordos

P3

Auburn University

Methane is produced in large quantities (natural gas) and can serve as feedstock for commodity chemicals. Activation of the C-H bond of methane is the first step for such chemical processes and is usually the rate-determining step since the C-H bond of methane is one of the strongest C-H chemical bonds. In this study, we examine the possibility of activating methane using metal anionic centers. Specifically, we perform Density Functional Theory (DFT) calculations to investigate the reaction of methane with Cu-, Co-, Ag-, Au-, and Ir-. We optimized the geometries of adsorbed species as reactants, transition states, and the various possible products. Our results show that Cu- and Co- can form stable HCuCH3- and HCoCH3- compounds, albeit via high activation barriers, while Ag- and Au- cannot. Interestingly, Ir- formed a much more stable product H4IrC- beyond the HCuCH3- as observed in others. These observations are in agreement with the experimental photoelectron spectra recorded for the products of the studied reactions. All calculations were performed using Gaussian 16 with the exchange-correlation functional B3LYP and the aug-cc-pVTZ basis sets. Relativistic effective core potentials were used for Au and Ag combined with the appropriate aug-cc-pVTZ-PP basis sets. Vibrational frequency calculations were used to confirm that the transition states bear a single imaginary vibrational frequency, and that reactants and products bear only real vibrational frequencies.

Characterizing the minima of the homogeneous trimers, tetramers and pentamers of hydrogen bromide and hydrogen iodide: (HBr)m and (HI)m where m = 3 - 5

Yuan Xue* and *Gregory S. Tschumper

P4

The University of Mississippi

With an expanded valence treatment that includes dynamical electron correlation for the subvalence (n - 1)d electrons for Br and I, this work characterizes the minima of homogeneously hydrogen-bonded (HBr)m and (HI)m clusters where m = 3 - 5. All minima and low-lying transition states reported herein were fully optimized utilizing the MP2 ab initio method and the B2PLYPD double hybrid functional with empirical dispersion corrections. These computations were conducted with the triple-ζ polarized correlation consistent basis sets augmented with diffuse functions. CCSD(T) optimizations were also carried out on candidates for the global minima and select transition states. They are denoted aCVTZ and consist of aug-cc-pVTZ for H and aug-cc-pwCVTZ-PP for Br and I, where the 10 and 28 inner-core electrons, respectively, were replaced with the corresponding MDF pseudopotential. The nature of the stationary points was verified with harmonic vibrational frequency computations at the same level of theory. Our CCSD(T) computations indicate that the global minima of the homogeneous trimer, tetramer and pentamer systems are hydrogen-bonded cyclic structures with C3h, S4 and C1 point group symmetry, respectively, for both HBr and HI. At the CCSD(T)/aCVTZ level of theory, the electronic dissociation energy (De) for the (HBr)3, (HBr)4 and (HBr)5 minima are ca. 6.4, 9.9 and 13.0 kcal/mol and the De for the (HI)3, (HI)4 and (HI)5 are ca. 5.5, 8.7 and 12.2 kcal/mol. Interestingly, the C4h configuration of (HBr)4 and (HI)4 are found to be low-lying transition states that are respectively ca. 0.15 and 0.65 kcal/mol higher in energy compared to the corresponding S4 minima at the CCSD(T)/aCVTZ level of theory. A few additional minima have also been identified for trimers, tetramers and pentamers of both HBr and HI, but further computations indicate that they all have higher electronic energies than the aforementioned global minima.

Multiscale Shock Technique Approach for Investigating the Orientation-Dependent Structural Evolution of α-Quartz Under Shock Compression

Huadian Zhang*, *Yuan Xue*, *A.M. Rajendran*, *Manoj K. Shukla*, *Steven Larson*, *and Shan Jiang

P5

University of Mississippi

The structural evolution of α-quartz under shock compression is of significant interest due to its ability to transform into various polymorphs, offering insights into shock metamorphism. In this study, we present a molecular dynamics investigation of the anisotropic shock response and mechanical behavior of α-quartz single crystals using the multiscale shock technique (MSST). Compared to conventional non-equilibrium molecular dynamics, MSST enables the simulation of atomistic processes at the shock front over extended time scales, which is essential for capturing the kinetics of structural changes and anisotropic mechanical responses. Simulations along the [100], [120], and [001] crystallographic orientations reveal that shock-induced phenomena—including the Hugoniot elastic limit (HEL) and polymorphic transformations—are highly orientation-dependent. Notably, a "two-wave" feature in the shock Hugoniot relationships indicates complex structural transitions prior to strong shock loading, consistent with previously reported experimental data. Detailed analysis of atomic configurations shows that certain orientations retain crystallinity under shock, while others undergo amorphization, highlighting the dynamic interplay between crystal structure and shock response. Unloading tests further support the presence of residual elasticity in shocked α-quartz, confirming the partial preservation of crystalline properties prior to structural breakdown. While the MSST approach, when combined with the bond-order Tersoff potential, enables efficient simulation, it exhibits limitations in accurately predicting density and certain polymorphic structures. To address these issues, schemes have been proposed that utilize machine-learned interatomic potentials trained on density functional theory (DFT) data. Alternatively, some approaches employ ab initio molecular dynamics directly. Preliminary results demonstrate the feasibility of using MSST with ab initio molecular dynamics to simulate polymorphic transitions in α-quartz, paving the way for optimizing the Tersoff potential parameters. This synergy between MSST and advanced interatomic potentials is critical for unraveling complex atomic-scale mechanisms governing material response under high-pressure conditions, with broad implications for materials science and engineering.

A Photochemical Crossroads: The (Z)/(E) Equilibrium Determines Emission or Cyclization of 2'-Hydroxychalcone

Peyton D. Simpson*, *Matheus M. F. de Moraes*, *Megan J. Mackintosh*, *Lee M. Thompson**, *and Pawel M. Kozlowski*

P6

University of Louisville

The molecule 2'-hydroxychalcone (2HC) exhibits unique photoprocesses, including excited-state proton transfer and photoisomerization. While many of the major components of the photochemistry of 2HC have been reported previously, there remains a lack of consensus concerning the importance of the proton transfer step and its contribution to the isomerization. Herein, we employed second-order n-electron valence state perturbation theory (NEVPT2) to investigate the potential energy surfaces of 2HC's low-lying singlet and triplet excited states with several key reaction coordinates, focusing on the mechanism for the photoisomerization and emission. Our results exhibited excellent agreement with previous experimental studies and are qualitatively consistent with previous theoretical works but provide a more accurate modelling of the excited states. Additionally, we investigate the importance of the equilibrium between the (Z)-keto and (E)-keto isomers in the ground state which was not considered in previous works. The excitation of the (Z)-keto and (E)-keto leads to distinct photochemical reactions where the photochemistry of the former involves fluorescence and phosphorescence while the latter involves a photocyclization via a conical intersection. This improves the current understanding of the photochemistry of 2HC that can be extended to spectral tuning to enhance or inhibit fluorescence and cyclization of 2HC and its derivatives.

Theoretical Spectroscopic and Thermodynamic Properties of the UX0/-/+ (X = Li and Be) and Comparison of the U Atom Binding to 2nd Row Elements.

João Gabriel Farias Romeu*, *Gabriel F. de Melo*, *David A. Dixon

P7

The University of Alabama

Diatomic molecules containing actinides are of special interest as simple models for studying the f-element chemistry and due to their application in molten salt reactors. High-level correlated molecular orbital theory calculations at the CASPT2-SO and CCSD(T) levels were performed on the UX0/+/- (X = Li and Be) and WX (X = Li, Be, C – F), complementing the previous investigations across the 2nd row elements. The Feller-Peterson-Dixon (FPD) method and multireference CASPT2 calculations combined with spin-orbit effects were carried out to provide a reliable description of the electronic states, bond dissociation energies (BDEs), ionization energies (IEs), adiabatic electronic affinities (AEAs), and vertical detachment energies (VDEs). At the FPD level, the IE(ULi) is predicted to be 4.650 eV (ULi), which is lower than the IE(Li); the IE(UBe) is 5.901 eV, which is similar to the IEs of U, and UX (X = B – F) and consistent with the NBO analysis showing that the ionization process is governed by the loss of one U(7s) electron. The AEAs are 0.708 eV (ULi) and 0.989 eV (UBe), which are lower than those for UB, UC, UN, and UO; UF has the lowest AEA across the series. The electron addition to form UX- all occurs in the 7s orbital of U from UBe to UO; the same process occurs in the Li(2s) for ULi and in the U(6d) for UF. The FPD values for the BDEs are 37.7 (ULi) and 8.0 kJ/mol (UBe), and increase from UBe to UO; the BDE(UF) is lower than the BDE(UO), but higher than the BDE(UN). For the WX (X = Li – F) series, the BDEs(WX) are larger than the corresponding BDEs(UX) from Li to N, and switch for O and F due to the higher ionic character of the monoxides and monofluorides and the higher IE of W than U. This work was supported by the U.S. Department of Energy (DOE), Office of Science, Office of Basic Energy Sciences, Heavy Element Chemistry program through Grant No. DE-SC0018921.

Theoretical Electronic Spectroscopy of Gas Phase Transition Metal Acetylide Cations (MCCH+, M = Sc,Ti, ... ,Zn)

Haritha K Sasi*, *Nathan J DeYonker

P8

University of Memphis

CCH radicals are among the abundant interstellar polyatomic molecules predominantly observed in molecular clouds and planetary nebulae, while their anionic counterparts, C_2H^-, are considered a plausible component in the Interstellar medium (ISM) but have not yet been detected. Via fundamental metal-carbon bonding, MC2H molecules exhibit strong polarity, enhancing the intensity of their rotational transitions and improving the chances of astronomical observation. In this study, highly accurate single reference coupled cluster theory [CCSD(T)] is compared to multireference configuration interaction theory (MRCISD+Q) to survey the electronic structure of 3d metal mono acetylide cations (MCCH+, where M = Sc to Zn) which could catalyze gas phase reactions cold astrochemical environments. Theoretical characterization of the ground and excited electronic states of these specific ions will assist in their astronomical detection, constrain laser spectroscopy experiments of the neutral species, and guide characterization in synthetic labs. The study concludes, the variationally accessible states of $MCCH^+$ arise from interactions between the ground state of the ($^1\Sigma^+$) C_2H^- and the metal di-cation (M^{2+}). A thorough analysis of potential multireference characters of these states is reported. Harmonic vibrational frequencies, infrared intensities, and dipole moments are also reported for the identified ground states.

PlasMol: A Robust Software Interfacing Classical Electrodynamic Simulations with Quantum Mechanical Calculations

Brinton Eldridge*, *Daniel R. Nascimento*, *Yongmei Wang

P9

University of Memphis

The interaction between plasmons and molecules at the nanoscale plays a pivotal role in various light-matter phenomena, driving advancements in fields such as spectroscopy, nanolasers, and solar cells. Despite its significance, accurately simulating these interactions remains challenging due to the complex interplay between electromagnetic and quantum mechanical effects. To address this challenge, we propose the development of PlasMol, a novel software tool designed to simulate plasmon-molecule interactions with high fidelity and accessibility. PlasMol integrates Finite-Difference Time-Domain (FDTD) simulations for the electromagnetic response of plasmonic nanoparticles with Real-Time Time-Dependent Density Functional Theory (RT-TDDFT) for the quantum mechanical response of dye molecules. The tool prioritizes modularity and interoperability, allowing seamless integration with various quantum chemistry software packages. By combining state-of-the-art computational methods with user-friendly Python-based implementation, PlasMol aims to provide researchers with a versatile and open-source platform for studying complex light-matter interactions at the nanoscale.

Continuous Local Symmetry from Electronic Structure Theory

Duc Anh Lai*, *Devin Matthews

P10

Southern Methodist University

Symmetry serves as a central driving force for many branches of modern chemistry, including material science, synthesis, catalysis, and spectroscopy. While a chemical system may exhibit a high degree of long-range order, hidden symmetry deviations at local sites can significantly influence its molecular properties. From this perspective, the degree of symmetry continuously varies throughout the entire system, with some regions being more or less symmetric than others. In ab-initio structure theory, basis functions are used as elemental blocks to determine the molecular energy and construct quantum states, from which molecular properties are derived. Therefore, localized properties of a system are inherently encoded within individual basis functions rather than within the total wavefunction. By applying symmetry operations to subsets of basis functions, we measure changes in electron density to quantify local symmetry at any point, from which an iso-surface is constructed to represent the distribution of symmetry within the molecular environment. This continuous local symmetry measurement is capable of identifying non-symmetric centers. Furthermore, we show that the site symmetry values correlate with data observed in molecular spectroscopy. Finally, we demonstrate how the method can be used to elucidate the local chirality in chemical systems.

Combining Focal Point Geometries and Zero-Point Vibrational Energies with Higher-Order Corrections to Compute Experimental Binding Energies of van der Waals Dimers

Luke A. Kurfman*, *Jaden C. Yon*, *Philip M. Nelson*, *C. David Sherrill

Georgia Tech

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The binding energy of a dimer is a key experimental result that can be used to benchmark different levels of electronic structure theory and their ability to match spectroscopy studies. A variety of approaches using DFT, MP2, and coupled cluster methods have been utilized to replicate existing binding energies, employing different levels of theory to optimize the geometry and calculate the zero-point vibrational correction to the electronic energy. Such methods often yield accurate binding energies and illustrate their viability as cost-effective procedures that can be employed on larger clusters. However, many studies shy from employing more than the MP2 level of theory for geometry optimization, raising the question if a coupled cluster geometry could be used to obtain energies consistently within chemical accuracy or even 1 kJ/mol. Thus, the goal of this study is to utilize as high of a level of theory as possible to calculate accurate binding energies for dimers of small molecules. A focal point approach, combining CCSD(T)/aug-cc-pV(D+d)Z and MP2/aug-cc-pV([T,Q]+d)Z, was employed to optimize the dimer geometries. The same approach was used to obtain the frequencies and zero-point vibrational correction to the electronic energy. A similar focal point approach that adds an additional level of basis set to each energy, alongside counterpoise and core-valence corrections, was then employed to obtain the electronic energy, allowing us to compute the binding energy of multiple dimers. Additionally, we evaluated the importance of multiple higher-level corrections, including diagonal Born-Oppenheimer, scalar relativistic, vibrational anharmonicity, and CCSDT(Q) corrections.

Distance and Orientation Dependence of Triplet-Triplet Energy Transfer Couplings Based on Nonorthogonal Multireference Wave functions

Saptarshi Saha*, Megan J. Mackintosh, Lee M. Thompson,* and Pawel M. Kozlowski **P12**

University of Louisville

Triplet-triplet energy transfer (TEnT) has significant contributions in different photochemical, photobiological, and energy science processes. The best-known form of TEnT is the Dexter energy transfer (DET). DET is well described by the four-state model which includes initial and final states (D*A and DA*) as well as charge transfer (CT) states (D+A- and D-A+). Two model systems, namely naphthalene dimer and the 2,2'-bifluorene molecule were utilized to investigate the role of distance and orientation of the molecular fragments on the energy transfer process. For naphthalene dimer, in D2h symmetry, x, y and z distances (in Å between the naphthalene monomers were varied and the electronic coupling elements (ECEs) plotted corresponding to them. Maxima in the ECE curves were seen corresponding to regions of greatest π and π^* orbital overlap, whereas minima were observed along π orbital nodes. For 2,2'-bifluorene, the variation of ECEs was studied with respect to the torsional angle between the two fluorene rings connected through the C2-C2 bond. Spin density plots and biorthogonal orbitals were used to verify that the correct diabatic electronic structure of the TEnT states were determined. As a future direction, we will extend our investigations to determine the importance of TEnT pathways in various photosensitized catalytic reactions and other applications.

Ion-gated two-dimensional membranes for gas separation

***Yujing Tong*, Dr. Hongjun Liu, Dr. Shannon M Mahurin, Porf. Sheng Dai and Prof. De-en Jiang**

P13

Vanderbilt University

Ionic gating has emerged as a powerful strategy to regulate pore sizes in 2D materials, enabling precise control over gas transport for molecular separations. In this work, we explore two classes of ion-gated membranes—multilayer porous graphene and quasi-tetragonal-phase (qTP) fullerene networks—for high-performance gas separation. Molecular dynamics simulations reveal that introducing ionic liquids between graphene layers dramatically enhances CO_2/N_2 selectivity (up to $\sim$795) while maintaining high CO_2 permeance, due to stabilized anions that effectively turn the pore size to 3.3–3.6 Å. In parallel, ion-gated qTP fullerene membranes demonstrate exceptional O_2/N_2 separation performance. Ion size and position are shown to refine effective pore size, with qTP1-Li achieving a selectivity of 93 and permeance surpassing 5×10^5 GPU. These studies highlight ion gating as a versatile approach to engineer dynamic sieving effects, offering design principles for next-generation membranes that break the permeance–selectivity trade-off for gas separation applications.

Description of Excitations in Molecules using Factorized Electron-Nuclear Dynamics

Julian Stetzler*, *Sophya Garashchuk*, *Vitaly Rassolov

P14

Univeristy of South Carolina

An accurate yet efficient approach for simulating the dynamics of electrons and nuclei in large systems (100s-1000s of atoms) is a major challenge for theoretical chemistry. Recently, we have developed a new approach based on the exact factorization of the electron-nuclear wavefunctions, which utilizes an effective complex potential for simulating the dynamics of electrons and nuclei without referencing the electronic energy eigenstates. Moving beyond analytic models, we implement the method and study its stability and accuracy for the dynamics of the H2+ molecular ion in a laser field. I will present the systematically improvable numerical approximations necessary for a robust method of quantum electron/nuclei dynamics under development in the group. With that, we will be able to analyze performance of the standard electronic structure methods in the context of the electron-nuclear dynamics involving large number of electronic excitations. Specifically, we will investigate the effects of the electronic basis size on derivative coupling terms and nuclear dynamics. Specifically, we will investigate the effects of the electronic basis size on derivative coupling terms and nuclear dynamics.

Dynamics with Quantum Trajectory Guided Adaptable Gaussian bases

Michael Anim Safo* and *Sophya Garashchuk

P15

University of South Carolina

The incorporation of nuclear quantum effects (NQEs), such as tunnelling, zero-point effects, and transitions between different electronic states in quantum dynamics, has gained much interest in physics and chemistry. However, traditional methods that describe these unique effects are limited to a few dimensions due to exponential scaling of wavefunctions with the system size. We present the ongoing development of an efficient trajectory-based method, known as Quantum Trajectory Adaptable Gaussian Bases (QTAG), implemented in the modular software library Libra, which offers improved scalability for higher dimensional molecular dynamics. The QTAG method currently invokes a global fitting procedure for computing trajectory momenta across all basis functions. This procedure may encounter singularities near the nodal regions of the wavefunction leading to unstable trajectory dynamics. Herein, we present a novel procedure, where each momentum is fitted semi-locally within a gaussian window function whose spatial localization is controlled by a single parameter within a weighting function. This approach circumvents issues associated with singularities near nodal regions of the wavefunction. The approach is applied to benchmark systems including the nonadiabatic Tully Model (I and II) and the Holstein model to assess the regime of applicability, and to evaluate the performance of the new procedure of evolving the QTAG basis and the accuracy of the ensuing quantum dynamics.

Revealing correlation mechanisms through nonorthogonal multiconfiguration self-consistent field calculations

Zihui Song; Jonathan S. Bersson ; Lee M. Thompson **P16**

University of Louisville

Building on the “different orbitals for different configurations” framework, the non-orthogonal multi-configuration self-consistent field (NOMCSCF) method has been developed to simultaneously optimize both molecular orbitals and configuration interaction (CI) coefficients. While NOMCSCF calculations can be initialized from a set of arbitrary nonorthogonal determinants, such as a set of local minima in self-consistent field (SCF) solution space, they can instead start from an orthogonal expansion, such as that obtained from a complete active space (CAS) expansion. Unlike orthogonal based optimization of orbitals over the CAS expansion (CASSCF), which primarily captures static correlation, NOMCSCF also accounts for differential dynamic correlation by allowing each configuration to adopt its own optimized set of orbitals. In this presentation, I will discuss how spin and spatial symmetry constraints can be applied to the orbital optimization within the NOMCSCF framework. I will present results that demonstrate how symmetry constraints affect the energies and properties of the resulting NOMCSCF wavefunction, even when the overall wavefunction remains spin-adapted. Notably, I will illustrate how symmetry constraints reveal the correlation mechanisms that act between orbitals, with application to active space partitioning approaches.

Beyond non-orthogonal wave functions: Recovering correlation energy via perturbation theory for applications in excited-state processes

Megan J. Mackintosh, Lee M. Thompson **P17**

University of Louisville

Photoreactions catalyzed by transition metal complexes can involve a competition between photoinduced electron transfer and excitation energy transfer pathways which can result in different chemical outcomes. Theoretical approaches can provide insights into such photoreactions. However, in the context of wave function based methods, modelling of transition metal catalysts with high-accuracy typically involves very large expansions which are not computationally expedient. To overcome this challenge, non-orthogonal configuration interaction (NOCI) models have proven useful computational tools due to their “different orbitals for different configurations” picture allowing for very compact wave functions which is especially useful for modelling excited states. Despite this advantage, it is still necessary to recover the dynamic correlation energy. To address this, we seek to apply the MP2 method in conjunction with the NOCI approach to the simulation of excited state processes including photoinduced electron transfer and excitation energy transfer. More specifically, we are developing multi-reference implementations of MP2 theory which are based on a perturb-then-diagonalize scheme involving an effective Hamiltonian. We will describe our progress towards implementing such strategies within the NOCI framework.

Ab initio design of new 2-dimensional electrides with hybrid electronic structures

***Andrei Evdokimov**, Valentina Nesterova, Marcelo Kuroda, Konstantin Klyukin, Evangelos Miliordos*

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Auburn University

Solvated Electron Precursors (SEPs) are metal-ligand complexes featuring peripheral diffuse electrons that exhibit distinctive pseudoatomic electronic structures. These unique characteristics underpin their promising roles in quantum computing applications and capture and utilization of CO2. Here we introduce novel family of electrides, where SEP molecules are anchored to surfaces, which we term Surface Immobilized Solvated Electron Precursor Electrides or SISEPEs. The adsorption of molecular species on the stable substrates is expected to help to achieve synthesizability of SEP-based material. Our ab initio study shows that by tuning the coverage density of SEPs on the surface, the electronic structure of SISEPEs can be varied from locally diffuse electrons to one-dimensional electronic channels and two-dimensional 'seas' of electrons while maintaining the constant chemical composition. This feature determines distinctive hybrid organic/inorganic electronic structure of SISEPEs, enabling to switch between organic electrides-like electronic structures (0D and 1D) and inorganic electrides-like electronic structures (2D).

Multireference equation-of-motion formalism based on the driven similarity renormalization group: theoretical foundations and applications to ionized states

***Zijun Zhao**, Shuhang Li, and Francesco A. Evangelista*

P19

Emory University

We present the first derivation and implementation of the equation-of-motion (EOM) extension of the multireference driven similarity renormalization group (MR-DSRG) formalism for ionization potentials (EOMIP-DSRG). The EOMIP-DSRG method can deliver accurate ionization potentials for systems with strong electron correlation at $O(N^5)$ scaling in the EOM step with the basis set size N, and also allows for efficient calculation of spectroscopic properties, such as transition intensities. We present three variants of the EOMIP-DSRG method, based on the iterative MR-LDSRG(2), and the perturbative DSRG-MRPT2/3 methods. The EOMIP-DSRG methods are used to calculate 1) the vertical ionization potentials of a series of small molecules at both equilibrium and stretched geometries; 2) the spectroscopic constants of several low-lying electronic states of the OH, CN, N2+, and CO+ radicals; and 3) the binding curves of low-lying electronic states of the CN radical. A comparison with experimental data and other theoretical results shows that all three EOMIP-DSRG methods are able to accurately reproduce the vertical ionization potentials and spectroscopic constants of these systems, with the ones based on DSRG-MRPT3 and MR-LDSRG(2) exceeding the accuracy of many state-of-the-art multireference methods with equal or higher computational scaling.

Language model-based chemical entity extraction tool for Chorismate Mutase enzymatic reaction

Saghar Gomrok*, *Qianyi Cheng

P20

University of Memphis

Computational approaches can effectively address the experimental limitations in studying enzymatic reactions. Despite computational advancements, accurately simulating enzyme reactions and ligand interactions remains a challenge. Furthermore, extensive enzymatic research data is often heterogeneous, dispersed across multiple sources, and difficult to access or interpret efficiently. In this study, we present an automated pipeline designed to systematically explore relevant publications on the enzymatic reaction of chorismate mutagenase and extract information. This organized knowledge serves as the foundation for the development of a quantum mechanics (QM) model, incorporating critical data such as essential residues, conformation information, and computational methods. The process begins with a domain-specific search engine that queries well-known scientific databases. Comprehensive metadata from retrieved articles, along with their references, cited publications, and full texts, if available, will be stored to enable subsequent similarity assessments and information extraction. Following the retrieval phase, the articles are ranked according to their relevance to the target enzyme reaction and the research objectives. Among all the tasks, Named Entity Recognition (NER) techniques are important to be fine-tuned into the chemistry domain, so that they can be better utilized to facilitate information extraction specifically targeting computational enzymology. To enhance accuracy in identifying chemical entities, pre-trained BERT language models are fine-tuned using the human-annotated CHEMDNER dataset. Further enhancement is achieved by domain-specific fine-tuning with annotated enzymology texts. Ultimately, the refined model integrates fine-tuned language models with rule-based and dictionary-based methods, optimizing the extraction of enzymatic reaction parameters and QM calculation methodologies. This comprehensive methodology aims to establish an efficient and systematic framework for designing QM models in computational enzymology.

Hydrolysis Reaction Pathways of Thorium Oxide Nanoclusters

Eddy M. Lontchi*, *David Dixon

P21

University of Alabama

le in the behavior of actinides, their environmental impact, and their use in the nuclear industry. We performed computational studies on the hydrolysis of thorium ThnO2n (n = 3 - 6) clusters at the DFT, MP2, and CCSD(T) level. The hydrolysis proceeds by physisorption of H2O, forming a Lewis acid/base adduct with binding energies between -15 to -22 kcal/mol, followed by a proton transfer to form hydroxides. The process is repeated until all oxo groups are hydrolyzed. The initial water physisorption energy of $\sim$ 21 kcal/mol is consistent across the cluster sizes and compares with experimental values for ThO2 surface. The hydrolyzed products are predicted to be energetically preferred over the physisorbed products, and the transition state barriers are relatively low. Reaction coordinates were generated to show the calculated physisorption energies, reaction barriers, and hydrolysis energies. The work is extended into investigating the gas phase acidities and aqueous acidities for the various thorium hydroxide species. This work was supported by the U.S. Department of Energy (DOE), Office of Science, Office of Basic Energy Sciences, Heavy Element Chemistry program at The University of Alabama through Grant No. DE-SC0018921.

Augmenting MACCS Keys with Persistent Homology Fingerprints for Protein-Ligand Binding Classification

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P22

University of Tennessee, Knoxville

Cheminformatics, aided by machine learning, has become a cornerstone of modern drug discovery. This is due to the developed molecular fingerprints that translate a chemical's structure into a machine-readable format. Traditional substructure representations, like MACCS Keys, record the appearance of predefined structural fragments; however, they ignore the compound's overall morphology. Topological data analysis (TDA) is an interdisciplinary field of research that uses persistent homology to evaluate the underlying shape of data, and it can be represented using a persistence diagram, landscape, barcode. When applied as a chemical representation, it reveals unique insights into the structure's form, represented by the homological features: connected components, rings, and cavities. Integrating topology-based descriptors into a classic cheminformatic fingerprint produces an enriched description vector, which yields a more holistic representation of the molecule and improves the prediction of the molecule's protein binding interaction. Our work combines persistence images (PIs) with MACCS Keys into a single topological substructure vector (TSV) fingerprint and individually tests its predictive performance on 19 ChEMBL protein-ligand datasets using the same multi-layered perceptron classifier (MLPC) architecture. Persistence images capture each molecule's intrinsic geometry and connectivity, while MACCS Keys encode chemical substructures. Across all but one dataset, the TSV descriptor outperformed its individual components, achieving the highest average validation Matthews correlation coefficient of 0.7988. In contrast, the MACCS Keys' score was 0.7075, and the TPI descriptor scored 0.7655. These results show that adding topology-based features to classic fingerprints can boost classification reliability in computer-aided drug design.

Torsion and substitution effects on singlet-triplet gaps in anti-Bredt olefins: a multi-reference study

Emily A. Huang*, *Francesco A. Evangelista

P23

Emory University

Anti-Bredt olefins (ABOs) are defined as bicyclic systems with a highly strained bridgehead double-bond. Originally thought of as inaccessible according to Bredt's 1924 rule, recently they have been indirectly observed in cycloaddition reactions by McDermott et al. ABOs are a promising reactive intermediate in cycloaddition reactions, deserving large-scale screening efforts. The reactivity of an ABO is related to its diradical character, with the singlet-triplet (S-T) gap being a directly measurable proxy. The vast majority of computational studies of ABOs utilize density functional theory (DFT). However, being highly strained, these systems are expected to exhibit varying degrees of strong correlation, which calls for a systematic multi-reference study of ABOs. In this work, the singlet-triplet gaps of a library of ABOs are assessed with the second-order multi-reference perturbation theory based on the driven similarity renormalization group (DSRG-MRPT2). The DSRG-MRPT2 values were generally found to be higher than the DFT values but following the same general linear trend with S-T gap plotted against the torsion angle of the bridgehead double bond. Substituted compounds were found to follow the same trend as the unsubstituted compounds, indicating that the torsion angle of the bridgehead double bond is the main contributor to the S-T gap.

Hydrogen Containing Halomethane Thermochemistry at the G3(MP2) Level. Heats of Formation, C-H Bond Dissociation Energies, and pKa Values.

Thomas Dalton Andress*, *Cole Seely*, *Vittorio Pace*, *and David A. Dixon

P24

The University of Alabama

The heats of formation, bond dissociation energies, proton affinities, gas phase acidities, and pKa values of all halomethanes containing hydrogen plus methane were calculated at the DFT, MP2, and G3MP2 composite MO levels. The G3MP2 method was extended for iodine containing compounds by using the aug-cc-pwCVTZ-PP basis set for I for the MP2 large calculation. The calculated gas phase acidities are in agreement with the available experimental data within the experimental error limits and many values are within 4 kJ/mol agreement. A notable exception to experimental agreement is CH2F2 which differs from our calculated value by nearly 40 kJ/mol for ΔG acidity. CCSD(T) with a complete basis set extrapolation predicts a value consistent with the G3MP2 value showing that these experimental values are incorrect. pKa values for the hydrohalomethanes range from 52.7 for CH3F to 26.9 for CHF2I using G3MP2. This study provides the most comprehensive and accurate heats of formation, C-H bond dissociation energies, gas phase acidities, and pKa values for the complete set of halomethanes containing hydrogen.

Atomic Polarizability: Investigating the Theory-Experiment Disagreement

Ajay Melekamburath*, *Edward F. Valeev

P25

Virginia Tech

Polarizability is a key property that underpins a wide range of phenomena in chemistry and materials science, from intermolecular interactions to optical responses. While numerous theoretical approaches exist for computing static and dynamic polarizabilities, significant discrepancies often persist between calculated and experimental values for certain elements. In this work, we focus on the Aluminum atom as a case study to systematically investigate the origins of these differences. Using both analytical and numerical techniques, we examine the impact of basis set selection, relativistic effects, and higher-order correlation on computed polarizabilities. Our ongoing work aims to identify the primary sources of disagreement and to provide guidance for improving the accuracy of theoretical predictions in atomic and molecular systems.

Computational Study of N-Hydroxylation Enzymatic Reaction

Anjali Arya* and *Qianyi Cheng

P26

University of Memphis

Cytochrome P450 (CYP) enzymes play an important role in the metabolism of drugs containing amine groups, by catalyzing N-hydroxylation reactions, which may lead to the formation of toxic metabolites. In this study, we revisit the CYP-catalyzed reaction pathways of aniline and mexiletine, focusing on the hydrogen atom transfer (HAT) and oxygen addition rearrangement (OAR) mechanisms. For aniline, 57 atom quantum mechanics (QM) cluster models were constructed to evaluate the HAT and OAR mechanism and to compare our results with those reported by Seger et al. (2015). Despite closely following their computational setup, we observed discrepancies between our results and theirs. These discrepancies suggest that small QM cluster models may be insufficient for accurately examining the reaction pathways and energetics, and that careful validation of the structures and their changes is needed. For mexiletine, molecular dynamics (MD) simulations were combined with QM-cluster modeling, and 10 QM-clusters were constructed based on selected frames from the MD trajectories. These models range in size from 440 – 431 atoms, and are expected to provide more reliable results for investigating the HAT and OAR reaction pathways.

AI4QC: Computational Chemistry Assistant for Quantum Mechanical Interaction Energies

***Austin M. Wallace*, Giri P. Krishnan, Remy Bondurant, and C. David Sherrill**

P27

Georiga Tech

Selecting an appropriate level of theory is a fundamental task in quantum chemistry, requiring a balance between accuracy and computational cost. While coupled-cluster singles and doubles with perturbative triples at the estimated complete-basis-set limit [CCSD(T)/CBS] delivers highly reliable interaction energies and properties, its expense often precludes routine use across many chemical applications. Consequently, quantum chemists must choose more affordable methods that remain sufficiently accurate. In this work, we develop predictive models for both compute time and error statistics for intermolecular interaction energies of small organic dimers. Compute times are modeled by fitting polynomials that reflect each method's formal scaling, and error estimates are generated using a message-passing neural network (MPNN) in the ΔAP-Net2 architecture, implemented in QCMLForge with PyTorch. ΔAP-Net2 models are trained on the BFDBext dataset—3052 dimers with 80 levels of theory including a CCSD(T)/CBS reference for interaction energies. These predictive models are integrated into AI4QC, a browser interface that accepts a dimer geometry and automatically generates an input file for the recommended level of theory, complete with predicted compute time and error statistics. By guiding level of theory selection, AI4QC will leverage numerical data to suggest optimal ways to run datasets, attempting to lower the barrier of required intuition and skills to effectively run QM calculations.

Evaluation of the Domain-Based Local Pair Natural Orbital Approximation Under the Many-Body Expansion for X23 Lattice Energies

***Jaden Yon*, David Sherrill**

P28

Georiga Tech

Lattice energies are a defining characteristic of organic crystalline materials that lead to the prediction of relevant physical properties. Under the many-body expansion (MBE), the computation of lattice energies degrades to computation of many-body interaction energies. Due to the simplicity of the underlying methodology, the MBE invites an exploration of the efficacy of various approximation methods in computing lattice energies to achieve high accuracy with minimal expense. Here, we investigate the performance of the domain-based local pair natural orbital (DLPNO) approximation for lattice energies within the X23 dataset. We consider the DLPNO approximation for both Møller-Plesset perturbation theory (MP2) and coupled-cluster singles, doubles, and perturbative triples [CCSD(T)] for direct comparison to their canonical counterparts, as well as to approach complete basis set coupled-cluster [CCSD(T)/CBS] lattice energy benchmarks. Preliminary results of dimer interaction energies show consistent agreement between DLPNO-approximated and full MP2, whereas DLPNO-CCSD(T) systematically underestimates short-range interactions compared to CCSD(T); full DLPNO-CCSD(T) lattice energies subsequently suffer similar errors. Future work will thus consider the effects of tightened PNO convergence cutoffs to yield better agreement with CCSD(T) as well as the inclusion of trimer interaction energies in achieving benchmark-quality lattice energies.

Automated implementation of spin-free high-order coupled-cluster methods

Azam Besharatnik*, *Edward F. Valeev

P29

Virginia Tech

For the practically-important case of closed-shell states the coupled-cluster equations should be solved in their spin-free form. Spin-free coupled-cluster methods (with 3- and higher-body clusters treated iteratively) can be done by integrating the spin out of the spin-orbital equations, or by starting from the spin-free ansatz. Unfortunately, the former is difficult to generalize to arbitrary ranks, and the latter suffers from the redundancy introduced by the lack of orthogonality and linear independence of spin-free excited manifolds. Here we present a general-order spin-free implementation of closed-shell coupled-cluster equation using the biorthogonalization approach of Knizia and Wang [1]. By removing terms related by permutational symmetry the resulting CCSDT R3 and CCSDTQ R4 equations contain 93 and 149 respectively, which is significantly more compact than the equations of Knizia and Wang and involves greatly reduced number of permutations than the naive approach we used earlier. High-performance parallel implementation is demonstrated within the Massively Parallel Quantum Chemistry package [1] by using the SeQuant package for symbolic derivation, spin-tracing and biorthogonalization, factorization and numerical interpretation of the equations via the TiledArray tensor framework.

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Introducing Ionization Potentials to Cluster Perturbation Theory

Malachi Kent*, *Filip Pawłowski

P30

Auburn University

Cluster Perturbation (CP) theory systematically approximates Coupled Cluster (CC) models to increase computational efficiency without sacrificing accuracy. CP theory shows promising results for calculating both ground state and excited state energies, however, ionization potentials (IP) have not yet been explored. CP theory introduces the CC parent state Jacobian partitioning and perturbatively adds corrections that approximate the CC target state. In other words, if no perturbative approximations were introduced then these models would be equivalent to the CC target state, or in the case of excitation energies (EE) and ionization potentials (IP) to EE-EOM-CC and IP-EOM-CC, respectively. CP theory differs from Møller-Plesset (MP) perturbation theory and CC perturbation theory (CCPT) in two major points. Firstly, it uses a similarity-transformed fluctuation potential with respect to the parent-space cluster operator. Secondly it employs the full parent-space Jacobian, as opposed to orbital-energy differences, in solving amplitude equations. Both these traits make CP series convergent in the difficult cases where MP and CCPT series diverge and allow CP to easily obtain molecular response properties, while maintaining a low computational cost.Our new, CP third order perturbation model approximating the IPs in the singles-and-doubles space, IP-CPS(D-3), is compared to IP-EOM-CCSD data.

Thermodynamics for the Hydrogenation of Carbonyls.

Damian P. Duda*, *Sarah Sprouse*, *and David A. Dixon

P31

The University of Alabama

This work presents a unified computational study of different hydrogenation reaction paths (see Figure) for a wide range of carbonyl compounds relative to hydrogenation catalysis. The free energy of solvation of the proton in acetonitrile (MeCN) and tetrahydrofuran (THF) was predicted at the G3MP2 level with explicit solvent molecules and implicit self-consistent reaction field calculations at the COSMO and SMD levels. The SMD model with two solvent molecules, produced results that align closely with the available experimental data. These solvation energies were integrated into a thermodynamic cycle to assess three distinct hydrogenation pathways for a range of carbonyl compounds, including aldehydes, ketones, carboxylic acids, esters, and amides. The study compared direct H2 addition (A) with two-step mechanisms involving either hydride transfer followed by protonation (B) or vice versa (C). Gas-phase reaction energies computed via G3MP2 were adjusted by the solvent corrections, revealing how electronic factors, substituent effects, and solvent interactions govern hydride affinities and protonation energetics. This work was supported by the U.S. Department of Energy (DOE), Office of Science, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences and Biosciences, and Catalysis Program on a subcontract from Pacific Northwest National Laboratory.

A study of excited state dynamics of atomic collisions: Non-adiabatic trajectory surface hopping

Megan Simons*, *Daniel R. Nascimento

P32

University of Memphis

Atomic collisions are important for understanding the composition and behavior of matter at the atomic level. They have many applications such as fusion reactions and research in physical chemistry and astrochemistry. Thus far, considerable efforts have been directed toward developing methods for describing atomic collision processes that are electronically adiabatic, where it can be assumed that nuclear motion follows a single potential energy surface. However, non-adiabatic behavior is both common and important in atomic collisions, such as thermal energy collisions. Therefore, this study investigates atomic collisions utilizing surface hopping molecular dynamics simulations, where a stochastic algorithm is employed that determines when the path of the nuclei (a trajectory) "hops" from one potential energy surface (PES) at a particular electronic state to another. In this work, we investigated the probability of atomic collisions between various small molecules and an O+ ion utilizing the Surface Hopping including ARbitrary Couplings (SHARC) program with the ORCA interface. We used configuration interaction singles (CIS) and time-dependent density functional theory (TD-DFT) computational methods for the excited state dynamics simulations. Our data demonstrates that an increase in the number of initial conditions and an increase in the simulation time is important in capturing all the electronic states and their behavior for each interaction.

Explicitly correlated electronic wave functions improved: Revising one- and two-particle basis lengthscales

Samuel R. Powell*, *Edward F. Valeev

P33

Virginia Tech

The slow basis set convergence of electron correlation energies obtained with conventional Slater-determinant based wave functions makes basis set incompleteness error (BSIE) a dominant source of error in ab initio electronic structure calculations1. Explicitly correlated (F12) methods speed up the basis set convergence by improving the description of the wave function at short interelectron distances2. Robust, high-quality F12 computations are conventionally known to require the inclusion of diffuse atomic orbitals (AOs) in the atomic basis for optimal performance. However, the inclusion of diffuse AOs contributes to poor numerical conditioning, which is especially problematic for large systems such as materials models or biological molecules. We explore the importance of these diffuse orbitals using a dual-basis implementation of the explicitly correlated coupled cluster singles and doubles (CCSD-F12) method, comparing their contributions to the conventional and explicit correlation energies. We conclude that the diffuse AOs contribute significantly to both energy components but have an outsized relative impact on reducing BSIE for explicitly correlated calculations due to the improved many-particle basis afforded by the F12 contribution. Furthermore, we show that the F12 results can be notably improved by reoptimizing the geminal lengthscale, as the recommended values obtained at the MP2-F12 level of theory are poorly suited for CCSD-F12 calculations. Optimizing the geminal exponents reduces the impact of diffuse AOs on the F12 energy, reflecting the different lengthscales of dynamical correlation addressed by the inclusion of diffuse AOs and F12 geminal terms.

Testing and expanding the capabilities of the RINRUS software package for building reliable and predictable QM-cluster models

Dominique A. Wappett*, *Nathan J. DeYonker

P34

The University of Memphis

QM-cluster modeling is commonly used in the field of computational enzymology, but the lack of widely accepted standards for selecting and representing amino acid residues limits the reproducibility of many studies. The RINRUS (Residue Interaction Network ResidUe Selector) toolkit automates, and thus simplifies, the process of building reliable and predictable QM-cluster models of enzymes. The user defines the "seed" of the model (the substrate and, where relevant, important cofactors and amino acid residues), and the active site residues are selected and truncated based on either their interatomic van der Waals contacts with the seed or distance from the seed. This presentation discusses recent work on calibrating and improving the RINRUS methodology and demonstrates useful new features of the software.

Reproducibility and predictability are key goals guiding the development of RINRUS. We have recently added a test suite to the code containing all combinations of the atoms within each canonical amino acid residue (over 42 million combinations in total) to ensure the robustness and consistency of the trimming procedure. This provides our team with a simple way of validating the trimming procedure against new capabilities of the software. Users will thus have clear expectations of how residues will be represented in the enzyme models they create with RINRUS.

Initial usage of RINRUS has focused on van der Waals contacts as a metric for selecting and ranking the priority of the active site residues. More recently we have seen that using F-SAPT interaction energies to re-rank the residues identified as having contacts with the seed (which we refer to as the first interaction shell) leads to better convergence of the thermodynamic and kinetic values computed from the QM-cluster models. We are currently using F-SAPT to look beyond the first shell of active site residues to see if more distal fragments missed by a contact-based selection metric improve agreement between the QM-cluster model and experiment.

While interaction-based selection metrics are more efficient for creating reliable QM-cluster models than a purely radial approach, we have added new options for creating distance-based models with RINRUS. By comparing how the computed free energies converge with different ranking schemes—interatomic contacts, F-SAPT interaction energies and distances—we aim to combine all approaches into one multifaceted QM-cluster model building scheme.

Methods for Simulating Vibrational Circular Dichroism Including Dynamic Electron Correlation

***Brendan M. Shumberger*, Kirk C. Pearce, T. Daniel Crawford**

P35

Virginia Tech

We present the first analytic-derivative-based formulations of vibrational circular dichroism (VCD) atomic axial tensors (AATs) for second-order Moller-Plesset (MP2) perturbation theory and the configuration interaction method including single and double excitations (CISD). Our formulation applies the definition of an orbital derivative to the reference, singly excited, and doubly excited determinants to obtain a second quantized form of the wave function derivatives allowing us to compute overlaps between fully normalized MP2 and CISD derivative wavefunctions.

X-ray Photoelectron Spectroscopy and Hydrogen Bond Network Topolgies in Water Clusters

***Alexis Antoinette Ann Delgado*, Devin A. Matthews**

P36

Southern Methodist University

The abnormal properties of water, governed by hydrogen-bonded networks, give way to different phases of disordered and ordered microstructures. Although x-ray photoelectron spectroscopy (XPS) and x-ray absorption spectroscopy (XAS), provide insights into the local structure of water, some spectral features observed experimentally have yet to be reproduced theoretically. In this study, we employ equation-of-motion coupled cluster methods in conjunction with recently developed hybrid basis sets, built from off-the-shelf Dunning's correlation consistent bases, to compute XPS for water clusters (H2O)n (n = 1-10). Our focus is to assess the effectiveness of our hybrid (combining basis sets on one atom) and mixed (combining basis sets for different atoms) basis sets in CVS-EOMIP-CCSD and TP-CCSD computations for core-ionized states. This research aims to establish a protocol for deriving reliable theoretical estimates and computational protocols for XPS spectra of larger water clusters. This extension aims to isolate cooperative effects and deviations from ideal additive behavior, providing a detailed understanding of spectral features concerning the hydrogen bond network topology.

Coordination Chemistry of Ra^{2+} and Lr^{2+} H2O and N2 Clusters

Amanda Loudermilk*, *Sarah Sprouse, Kathleen Butler and David A. Dixon

P37

The University of Alabama

Recent advances in the 88" cyclotron at Lawrence Berkeley National Laboratory have led to the ability to study compounds of radium and lawrencium. Ra is found in nuclear reactor waste and is being used for targeted alpha therapy. Lawrencium, a synthetic element, is the last member of the actinide series. The ability of Ra^{2+} and Lr^{2+} to form coordination complexes with water and dinitrogen, $[M(H_2O)_n]^{2+}$, $[M(N_2)_n]^{2+}$, and $[M(H_2O)(N_2)_m]^{2+}$, for M = Ra and Lr and n = 1-6 and m = 1-2 has been studied at the density functional theory (DFT) B3LYP/(aug)-cc-pVDZ(-PP)/Stuttgart RSC 1997 ECP level and the correlated molecular orbital theory CCSD(T)/(aug)-pVNZ-DK3 level. The N2 stretch frequencies are predicted to increase slightly when bound to Ra^{2+} and show a much larger decrease when bonded to the open shell Lr^{2+}. H_2O is predicted to bind more strongly to the M^{2+} than does N_2. The ligand binding energies decrease as H_2O and N_2 are added. The binding of H_2O and N_2 is much stronger to Lr^{2+} than for Ra^{2+} due to the much smaller ionic radius for Lr^{2+}. This work was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences and Biosciences, Heavy Element Program.

Actinium and Nobelium Coordination Chemistry: A Comparison of Directly Identified Molecular Species Produced in Gas Phase Reactions with Computational Interpretations

Sarah Sprouse* and *David. A. Dixon

P38

The University of Alabama

The chemical behavior of elements at the bottom of the periodic table presents a significant challenge to traditional periodic trend expectations due to unusual and unexpected chemical properties caused by relativistic effects. Experimental data for these elements remain limited, making it difficult to fully grasp their distinct chemical characteristics. This is particularly true for the late actinide elements (Z > 100) and for the superheavy metals (SHEs, $Z \leq 104$), where experiments can only be performed one atom at a time. In this study, we compare the chemical behavior of actinium (Ac, Z = 89) and nobelium (No, Z = 102) dications when exposed to H2O and N2. The results of electronic structure calculations at the density functional theory (DFT) and correlated molecular orbital coupled theory coupled cluster CCDS(T) levels on Ac2+ and No2+ complexes are used to explain the experimental observations on nuclear reactions performed at the 88-Inch Cyclotron Facility at Lawrence Berkeley National Laboratory (LBNL). Ligand bond energies, molecular geometries, and electronic descriptors were obtained. The results show that both Ac2+ and No2+ react similarly with H2O, but significant differences were observed in the reactivity with N2. Additionally, the wide range of molecular species observed in this study accentuates the importance of computationally analyzing species formed in SHE chemistry experiments to better understand the chemical properties of these rare elements. This work was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences and Biosciences, Heavy Element Program.

Highly efficient implementation of linear response relativistic coupled cluster

Paweł Wójcik*, *A. Eugene DePrince III

P39

Florida State University

The coupled cluster (CC) methods are the cornerstone of modern computational chemistry. By granting an access to the systematically-improvable and size-extensive simulations of molecules, the CC methods provide the most reliable predictions of molecular properties, and interpretation of experimental data. The interactions of small to medium sized molecules with light, which are relevant in fields spanning as wide as biology, chemical analysis, and quantum technologies, are an example of application where the need for accurate modeling of chemical properties is necessary. This contribution presents a novel and highly efficient implementation of the linear response CC model. The efficiency is achieved thanks to the use of the highly parallelized TiledArray library for tensor contractions. The implementation works in the framework of relativistic formulation of the CC theory offering application of this efficient method to molecules containing heavy atoms.

Friday Session

Quantum Chemical Interpretation of Experimental Recorded Photo-Electronic Spectra of Uranyl Complexes

Taylor Gregory*, *Evangelos Miliordos

P1

Auburn University

In this work, we perform high-level electronic structural calculations to examine the low-lying excited electronic states and the ground states of UO2(CH3CO2) 2,3 complexes. These calculations include static, dynamic, and spin-orbit effects. The results are used to interpret and assign the peaks of these systems' photoelectron spectrum.

Assessing the Accuracy of Electronic Structure Methods for the Description of UV-Visible Light Absorption Intensity by Organic Molecules in Solution

Jorge C. Garcia-Alvarez*, *Samer Gozem

P2

Georgia State University

Numerous studies have examined electronic structure methods' ability to reproduce molecular light-absorption energies. While arguably as important as energies, comparatively few studies have addressed the intensities (probabilities) of the predicted transitions. We looked at the oscillator strengths (OSs or f-values) predicted by four wavefunction methods (CIS, TD-HF, EOM-CCSD, and LR-CCSD) and the time-dependent (TD) implementation of nineteen DFT functionals. These included eight pure, eight hybrid, and three long-range-corrected hybrid functionals. We also tested the Tamm-Dancoff approximation (TDA) for nine of the functionals. For all methods, transition dipole moments (TDMs) were obtained in the length, velocity, and mixed gauges. Different basis sets (Pople, Dunning, and Jensen's) were tested as well.

We compared the computations to 85 OSs derived from the experimental absorption spectra of 69 small organic molecules in solution. Most transitions in this comparison set come from conjugated molecules and have $\pi\pi*$ character. In the comparison, we account for the effect of the solvent on i) the molecular wavefunctions, by using different polarizable continuum model (PCM) implementations, ii) on the electromagnetic field driving the absorption, by modeling the cavity field acting on the molecules, and iii) on the light's energy flux, by multiplying experimental OSs (f_{exp}) times the refractive index of the solvent n.

OSs computed (f_{comp}) using the TDA, CIS, or EOM-CCSD exhibit a strong gauge dependence, which is diminished in linear response theories (TD-DFT, TD-HF, and to a smaller degree LR-CCSD). Overall, for TDA and the wavefunction methods, the length gauge reproduces experiments better. LR-CCSD, EOM-CCSD, and TD-DFT f_{comp} values have $\sim$10-20% MAEs relative to n f_{exp}. CIS and TD-HF present significantly larger errors. The TDA results in roughly twice the error of full TD. LR-CCSD and pure functionals' f_{comp} values present a 1:1 ratio with n f_{exp} while hybrid functionals systematically overestimate experimental OSs by a magnitude that increases with the $\%$ of HF exchange included in the functional.

Assigning Flavin's Difference-FTIR Spectral Bands in Multiple Redox States Using Implicit and Explicit Solvation Model Simulations

D.P. Ngan Le*, *Gary Hastings*, *Samer Gozem

P3

Georgia State University

Flavins are versatile cofactors that undergo different redox, chemical, and/or photophysical transformations depending on the protein they are bound to. A powerful tool available for studying their transformations is Fourier Transform Infrared (FTIR) difference spectroscopy, where changes in the FTIR bands relate to specific changes in flavin's bonding or its interactions with its neighboring environment. However, while the IR spectra of oxidized flavins are well-characterized, fewer computational and experimental studies have focused on characterizing the IR spectra of flavins in their reduced (semiquinone or hydroquinone) states. Here, we employ hybrid quantum mechanical/molecular mechanical (QM/MM) models with implicit solvation to compute vibrational frequencies and infrared intensities for a model flavin in its oxidized, anionic semiquinone, anionic hydroquinone, and neutral hydroquinone states. The water solvent configurations around the flavin are sampled with molecular dynamics for each state. These calculations are used with (semi-)empirically determined broadening and frequency-scaling factors to simulate difference spectra. These calculated difference spectra aid in assigning bands in experimental FTIR difference spectroelectrochemistry and step-scan data in the literature. A particular focus is on bands in the diagnostic 1350–1750 cm-1 range. The band assignments provided here for flavin in aqueous solution will provide a useful reference for interpreting bands in FTIR difference spectroscopy measurements, and computations, of flavoproteins in the future.

Tuning mechanisms for intersystem crossing in LOV2 vs LOV1 domains of Phototropins.

Stephen Ajagbe*, *Paulami Ghosh*, *Samer Gozem

Georgia State University

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Flavin's spectroscopic, photophysical, and redox properties are sensitive to its interactions with neighboring polar or charged groups. Flavin-binding proteins capitalize on this sensitivity to tune flavin's chemical reactivity and photochemistry. A fundamental understanding of this tuning mechanism is necessary for the design of novel flavoproteins. Photoactive flavoproteins such as Light-Oxygen-Voltage (LOV) domains have served as important scaffolds to tune photophysics through amino acid mutations, resulting in a series of engineered LOV-based proteins that optimize fluorescence, intersystem crossing, photoreduction, and/or adduct formation over a range of different timescales. To better guide future engineering efforts, we have recently employed hybrid quantum mechanical / molecular mechanical (QM/MM) models of LOV domains to study how intradomain electrostatics exert control over flavin's photophysics. In this work, we focus on a series of LOV1 and LOV2 domains from three different organisms; by simulating their spectroscopic properties, energies of low-lying singlet π, $\pi*$ and triplet n, $\pi*$ states, and electrostatic projection maps, we present a comparative study that sheds light on difference in LOV domain intersystem crossing efficiency in different organisms. We noticed that for LOV1 domains, unlike LOV2 domains, the TnN, $\pi*$ excited state is higher in energy than S1π, $\pi*$ state which corroborates the statement of various literature that LOV1 is less efficient for ISC than LOV2 domains. These models not only serve as a benchmark for applying multi-reference QM/MM models to study photophysics of flavoproteins, but also provide mechanistic insight useful for knowing how to better engineer fluorescent flavoproteins and/or singlet oxygen generators.

Multiple tuning mechanisms for intersystem crossing in LOV2 vs LOV1 domains of phototropins: All paths lead to the triplet state.

Paulami Ghosh*, *Stephen O. Ajagbe*, *Samer Gozem*

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Georgia State University

In the presence of varying electrostatic environments, the flavin chemical moiety exhibits unique sensitivities depending on the charge distribution around the characteristic isoalloxazine ring. This property is particularly highlighted in proteins that tune the environment of the chromophore capitalizing on this sensitivity for redox and photochemical reactions. Therefore, a fundamental understanding of the mechanisms by which proteins tune flavin chemistry is necessary for the design of novel flavoproteins. To study this property of flavin in proteins, scientists focus on physically observable behavior such as absorption and emission spectra or chemical reactivity. For such studies, photoactive flavoproteins (such as Light-Oxygen-Voltage (LOV) proteins) are significant, serving as probes of flavin's electrostatic sensitivity. Using domains in this class of proteins, we thus provide a comprehensive description of the sensitivity of flavin photophysics to intradomain electrostatics. We have simulated the UV/Visible spectra and calculated the relative stability of optically active first single excited state ($S_{1\pi,\pi^*}$) and triplet n_N, π^* state (T_{n_N,π^*}) states to present a comparative study of three LOV1 domains and their corresponding LOV2 domains. We noticed that for LOV1 domains, unlike LOV2 domains, the T_{n_N,π^*} excited state is higher in energy than $S_{1\pi,\pi^*}$ state which corroborates the statement of various literatures that LOV1 is less efficient for ISC than LOV2 domains. To support our observations, we studied the active sites of the six proteins and calculated their electrostatic projection onto the flavin chromophore. These results provide a correlation between the observed bathochromic shift and the electrostatic potential around the polar pteridine and non-polar benzene ring.

APEC-F 2.0: Implementing Automated QM/MM Modeling for Flavoproteins for Fluorescent Protein Simulations and Redox Potential Calculations.

Sarah Elhajj*, *Jacopo D'Ascenzi*, *Samer Gozem

P6

Georgia State University

QM/MM simulations have emerged as valuable tools to model photoreceptor proteins. Photoreceptor proteins, which absorb light and transmit it as a biological signal to regulate a physiological response, have found important biotechnological applications in bioimaging, optogenetics, biomedicine, and biosensing. Three main classes of photoreceptor proteins (LOV, BLUF, and CRY) belong to the ubiquitous family of flavin-binding proteins called flavoproteins. More generally, outside of photoreceptors, flavoproteins are encoded in 1–3% of the genes of prokaryotic and eukaryotic organisms and are typically enzymes. QM/MM models of flavoproteins typically treat the non-covalently bound flavin at the quantum chemical level as it constitutes the main locus of reactivity as well as the chromophore responsible for light absorption in the visible range. The remainder of the environment including the protein, solvent and ions are treated classically at MM level. However, the setup of QMMM models manually is time-consuming and requires advanced technical and chemical knowledge. In pursuit of the spirit of studying chemical and biological mechanisms of flavoproteins, there is an interest in implementing user-friendly software allowing for efficient, systematic and congruous modeling of the complex biomolecules. The efforts of automating such protocols has started with ARM (for Rhodopsins), which inspired us to follow the same path and automate APEC-F, an average protein electrostatic configuration for flavoproteins. In this poster, I plan to talk about our recent efforts in automating our multi scale QM/MM code for flavoproteins, which uses open-source software including GROMACS for MD and OpenMolcas/Tinker interface for the QM/MM geometry optimization of flavin inside an averaged protein environment constructed by superposition of MM environments surrounding the chromophore. Then, I will present how APEC is currently being used in for two applications: 1) the spectral tuning of flavin-binding fluorescent proteins derived from LOV domains, and 2) the calculation of relative energy of mutation to compute changes in redox potentials by integrating APEC-F 2.0 into a free energy cycle approach.

Development of Spin-Generalized Real-Time Projected Density Matrix Embedding Theory

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P7

Georgia Institute of Technology

Although spin dynamics is prevalent through multiple fields of science, the types of systems that be studied computationally are limited due to the 'curse of dimensionality.' To address this problem of computational expense, we are developing a real-time extension of projected density matrix embedding theory (RT-pDMET), a fully quantum embedding (QM/QM) method. We have extended RT-pDMET to a spin-generalized formalism, in which an electron can adopt states beyond only spin-up or spin-down. This enables direct simulation of complicated spin states under non-equilibrium conditions. We have also taken advantage of an embarrassingly parallel part of the algorithm, as RT-pDMET fragments a system into smaller, independent calculations. Our parallelized, spin-generalized RT-pDMET enables a description of complex spin phenomena in large-scale systems, with wide-reaching applications in the study of spin dynamics.

Insights Into the Electronic Structure of (Ti-CO2)- and (V-CO2)- Species

Alexandros Androutsopoulos* and *Evangelos Miliordos

P8

Auburn University

Global warming constitutes a hard nut to crack since human activities have caused the accumulation of greenhouse gases in the atmosphere and, by extension, the increase of Earth's average surface temperature. Carbon dioxide is among the gases in question, as the exploitation of fossil fuels on our planet has resulted in an increase in its atmospheric concentration. To mitigate this issue, scientists have examined the carbon capture and utilization (CCU) approach, in which carbon dioxide is captured and converted into high-value chemicals such as methane, methanol, and formic acid. As reported in our recent work, metal anions can be utilized for capturing CO2 and catalyzing its reaction with other substrates to produce commodity chemicals. Within this context, our study focuses on providing accurate mechanistic insights and energetics for the reaction between titanium/vanadium anions and carbon dioxide using high-level multi-reference methods. To the best of our knowledge, such a fundamental theoretical study is missing from the literature.

Selected CI for Lindbladian Superoperators: Avoiding the Cost of Full Diagonalization

Chinmay Shrikhande*, *Nicholas Mayhall

P9

Virginia Tech

The evolution of open quantum systems can often be modeled with the Lindblad master equation, where the non-Hermitian Lindblad superoperator (L) governs dissipative dynamics. Extracting the steady state and dominant decay modes is essential for characterizing the system's relaxation dynamics, which typically requires full eigendecomposition and becomes computationally expensive for large Hilbert spaces of 4^n dimension. We explore the use of a Selected Configuration Interaction (SCI) approach to construct an efficient variational subspace for L, enabling the systematic extraction of its most relevant eigenstates. By iteratively expanding the subspace with configurations that contribute significantly to the late time dynamics, our method accurately captures the steady state and slowest decay modes while avoiding the computational cost of full diagonalization. We benchmark our approach against direct integration and full eigendecomposition, demonstrating its scalability and accuracy in modeling dissipative quantum systems.

Conformational Sampling and Energetic Landscape of the GNMT-Catalyzed Methylation Reaction

Jonathan Epih*, *Qianyi Cheng

P10

The University of Memphis

This study investigates the catalytic mechanism of glycine N-methyltransferase (GNMT), which involves transfer of a methyl group from S-adenosylmethionine (SAM) to glycine, forming sarcosine and S-adenosylhomocysteine (SAH). To capture conformational diversity and reduce structural bias, quantum mechanical (QM) cluster models were constructed from multiple molecular dynamics (MD) frames of the GNMT–substrate complex. Activation energies were calculated for 40 such models, each with slightly different residue compositions determined by proximity-based selection (RINRUS). Despite variation in the included residues, differences in calculated activation energies did not correlate with residue set differences. Instead, energy variation tracked with conformational features of the active site geometry, demonstrating that initial protein-substrate conformation is the dominant factor influencing catalytic barrier predictions. To support this, statistical and machine learning techniques were employed to identify structural descriptors most predictive of activation energy, offering insight into how conformation governs reactivity for this system. These findings emphasize the importance of conformational sampling in enzymatic modeling and highlight that accurate energy estimates can be achieved without rigidly defined residue sets, offering implications for rational enzyme design and computational efficiency.

Energy Pivoting in Least-Sqaures Tensor Hyper-Contraction

Chao Yin, James H. Thorpe, Devin A. Matthews

P11

Southern Methodist University

Tensor Hyper-Contraction (THC) has gained significant attention for its potential to reduce the computational scaling of post-Hartree–Fock electronic structure methods. However, the accuracy and efficiency of THC critically depend on the selection of a pruned grid point set. Thus, constructing a high-quality grid is essential for the broader applicability of THC-based approaches. In this work, we present a novel grid pruning algorithm that selects grid points based on their individual contributions to the total energy. The proposed method demonstrates improved convergence behavior for both Coulomb and exchange energies when compared to the traditional Cholesky decomposition technique, evaluated across five molecular systems, three correlated wavefunction methods, and four basis sets. Moreover, the algorithm enhances the smoothness of potential energy surfaces even with a reduced number of grid points. These results highlight a promising direction for the continued development of low-scaling THC methodologies.

Influence of three body effects on Halogen bonding

Sharon Ochieng and Konrad Patkowski

P12

Auburn University

Accurate computational data and their insightful decomposition are both crucial for advancing the understanding of weak interactions, particularly in domains such as materials science and enzyme-ligand binding mechanisms. Benchmark datasets play a vital role in validating computational methods and guiding their development. In recent years, the halogen and chalcogen bonding types of interactions have gained significant attention. They involve attractive forces between electrophilic atoms and Lewis bases and are characterized by regions of positive electrostatic potential termed "σ-holes." This study introduces an extended dataset representing halogen bonding interactions in intermolecular trimers, focusing on the magnitude and influence of three-body effects on the halogen bonds. The dataset encompasses various halogens, offering 214 trimer structures. The benchmark two- and three-body interaction energy terms are computed at the CCSD(T) level close to the complete basis set limit. At the two-body level, a detailed SAPT analysis shows the dataset spans the electrostatic, dispersion, and induction regions of the ternary diagram. Overall, this work aims to provide a comprehensive dataset for halogen bonding interactions and use it to benchmark computational methods as well as understand the origins of two-body and three-body forces in such systems.

Scaling Reduction in Open-Shell CCSD(T) through Tensor Decomposition

Daniel P. Devore* and *Devin A. Matthews

P13

Southern Methodist University

The challenge of wavefunction-based quantum chemical methods, such as coupled cluster theory, stems from the rapid increase in computational cost with molecular size. In this work, we utilize non-antisymmetrized Goldstone diagrams to simplify the implementation of open-shell rank-reduced coupled cluster theory with single, double, and perturbative triple excitations (UHF-RR-CCSD(T)). The Singular Value Decomposition (SVD) method is applied via the Higher-Order Orthogonal Iteration (HOOI) algorithm to reduce the computational scaling of the triple excitation tensor, t_{ijk}^{abc}, thereby lowering the overall scaling of CCSD(T) from $\mathcal{O}(\mathcal{N}^7)$ to $\mathcal{O}(\mathcal{N}^6)$. This reduction is achieved using Tucker-3 decomposition, where the sixth-order excitation tensor is factorized as $t_{ijk}^{abc} = U_{ai}^{X} U_{bj}^{Y} U_{ck}^{Z} t_{XYZ}$, effectively replacing it with three auxiliary third-order tensors and a core third-order tensor. We introduce three techniques for computing the auxiliary tensors U_{ai}^{X} to account for the four spin cases of the triple excitation tensor.

Characterization of Thorium Oxocarbonyl Complexes with Electronic Structure Theory Methods

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P14

The University of Alabama

Density functional theory (DFT) and correlated molecular orbital CCSD(T) theory methods were used to predict the low-lying configurations of neutral and anionic ThOx(COy)z molecules. The geometries were computed using the hybrid exchange correlation functional B3LYP in conjunction with triple-zeta correlation consistent basis sets (cc-pVTZ-PP for Th and aug-cc-pVTZ for C and O). Single-point calculations were then performed at those geometries using CCSD(T) and a series of weighted core-valence basis sets (aug-cc-pwCVnZ for C and O and cc-pwCVnZ-PP for Th; n = D, T and Q). The electron affinities, vertical detachment energies, and bond dissociation energies were calculated at the extrapolated CCSD(T) CBS limit. The calculations show that the experimental PES spectra is complicated by numerous transitions. This work was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences and Biosciences, Heavy Element Program.

The multi-occupancy effect, a roadblock in wave function based methods, from transition metals to lanthanides

Matheus M. F. Moraes*, *Lee M. Thompson

P15

University of Louisville

The double d-shell effect is a well known problem for wavefunction based modeling of first-row transition metal containing systems. The standard definition of this effect is mainly practical, in short, it is the necessity to consider a second active d-shell in multireference calculations. Such a purely practical definition prevents the development of alternative and more efficient ways to account for this effect. On the other hand, the multi-occupancy definition proposed by Moraes and Aoto attempts to explain the root cause of the double-d-shell effect. Based on this alternative point of view, we developed an approach that relies on a balanced set of orbitals, the Partially Fixed Reference Space (PFRS) protocols, which maintains accuracy but is less costly. In this work we show that the multi-occupancy effect can be observed and must be considered in other chemical systems, focusing in particular lanthanide-containing systems. Additionally, we will explore how the coupling of the PFRS protocols with non-orthogonal approaches has the potential to both improve accuracy and reduce computational cost.

Signatures of Hydrogen Bonding in Soft X-ray Spectroscopy

Afifa Yousaf*, *Devin A. Matthews

P16

Southern Methodist University

X-ray spectroscopy involves the interaction of X-rays with matter to analyze materials' electronic structure and chemical composition. X-ray photoelectron spectroscopy (XPS) provides detailed information about the elemental composition, chemical states, and bonding environments at the atomic level. We intend to investigate these spectroscopic methods using computation-based equation-of-motion coupled-cluster methodologies. Our main interest is observing predictable shifts in the XPS spectra of small molecules due to hydrogen bonding, especially involving donor and acceptor oxygen atoms. In this study, we focus on gas-phase hydrogen-bonded dimers of small organic molecules such as water, alcohols, peroxides, carboxylic acids, etc., which are known for their ability to engage in diverse hydrogen-bonded structures. We examine the predictability of these shifts and discover important trends (and anti-trends) related to chemical structure. We hope this research will enhance our understanding of the effect of hydrogen bonding on soft X-ray spectra and its potential implications for molecular structure studies.

Molecular Engineering for Drug Innovation using Computational IntelligeNcE (MEDICINE)

Mohamed Abdelaty*, *Konstantinos D. Vogiatzis

P17

The University of Tennessee

Alzheimer's Disease (AD), characterized by cognitive decline and neuroinflammation, currently lacks treatments capable of halting disease progression. Traditional drug discovery approaches, including molecular dynamics (MD) simulations, are resource-intensive, limiting their use in large-scale virtual screening. In this work, we propose an innovative computational framework utilizing advanced machine learning (ML) techniques to predict protein-ligand binding energies directly from static molecular descriptors, significantly reducing computational costs. This approach was initially tested on NLRP3, a critical neuroinflammatory target in AD, using FDA-approved drugs from the ZINC database. Through virtual screening and molecular docking, representative ligands were selected, and binding energies were evaluated via MD simulations and Molecular Mechanics Generalized Born Surface Area (MMGBSA). Future directions include the integration of deep learning neural networks, particularly graph-based architectures, to enhance prediction accuracy and generalize applicability. Generative AI methods will further facilitate the discovery and optimization of novel therapeutic candidates. Ultimately, this project aims to significantly advance computational drug discovery capabilities, addressing urgent medical needs beyond Alzheimer's Disease.

Quantum Chemical Modeling of Reactions at the Metal/Liquid Interface

Chengyuan Shao* and *Jesse McDaniel

P18

Georgia Tech

We combine QM/MM and frozen density embedding (FDE) to propose a QM/FDE/MM embedding approach for metal/liquid interfaces. The QM region is the active system; the FDE region covers a large, "frozen" part of the solid environment, while the MM region covers solvent molecules. This approach aims to capture complex interfacial environments while maintaining computational feasibility. Our prototype implementations use PySCF for adsorbate/metal cluster (mol) and adsorbate/metal surface (pbc) systems. Preliminary benchmarks validate the methodology. Ultimately, we will apply QM/FDE/MM to applications in heterogeneous catalysis to investigate solvation effects.

Kinetically-constrained ring-polymer molecular dynamics for chemical reactions spanning the non-adiabatic to adiabatic regime

Victor Suarez*, *Joshua Kretchmer

P19

Georgia Tech

We extend the previously developed kinetically-constrained ring polymer molecular dynamics (KC-RPMD) method to allow for the direct simulation of systems spanning a wide range of diabatic coupling. This extension preserves favorable properties of KC-RPMD in the non-adiabatic regime, namely the correct description in the Marcus inverted regime, but switches away from the constraint at high diabatic coupling recovering the appropriate adiabatic description. We demonstrate that KC-RPMD simultaneously captures both adiabatic and non-adiabatic electron transfer rate constants for a range of spin-boson based model systems with excellent numerical agreement with Marcus theory.

Tracking Excitations: Orbital-Resolved Absorption Spectra from RT-CC Autocorrelation function.

Aparna Krishnan*, *Zhe Wang*, *Hakon E Kristiansen*, *Thomas Pedersen*, *T Daniel Crawford

P20

Virginia Tech

We apply real-time time-dependent coupled-cluster (RT-TDCC) methods to study field-induced electron dynamics in helium and water. Absorption spectra are computed via Fourier transforms of the time-dependent dipole moment and the autocorrelation function (ACF). Dipole decomposition using time-evolved T and Λ amplitudes reveals orbital-level excitation contributions and symmetry characteristics. Additionally, population analysis from the ACF tracks the evolution of ground-state character under varying field strengths, offering insight into excitation regimes. Together, these tools enable a detailed interpretation of electronic response beyond conventional spectral analysis.

Symmetry Projection on Quantum Computers: Shaping the Future of Hardware-Friendly Ansätze

Muhan Zhang*, *Ilias Magoulas*, *Francesco A. Evangelista

P21

Emory University

Quantum computers hold the potential to revolutionize quantum chemistry, opening new avenues to target highly entangled states that are in principle chemically intractable. However, current quantum devices are prone to errors, such as decoherence and operational noise. An attractive way to mitigate these errors is to rely on quantum algorithms based on hardware-friendly ansätze that give rise to quantum circuits with a substantially reduced number of two-qubit gates, which dominate the operational noise. Despite their usefulness from a hardware perspective, such ansätze typically break physical symmetries central to electronic structure theory. This symmetry breaking becomes especially problematic at crossings of potential energy surfaces with differing symmetry characters, causing variational quantum algorithms to fail in tracking target states. In this work, we address this issue by restoring good quantum numbers via symmetry projection. Specifically, we employ a variation-after-projection technique, allowing us to optimize parameters in the symmetry-adapted space, and restore particle number and spin symmetries. Our numerical simulations show that symmetry projection preserves these symmetries without a significant overhead of two-qubit gates, maintaining the efficiency of the original ansätze. Our results establish symmetry projection as a practical pathway for realizing hardware-friendly ansätze on noisy and fault-tolerant quantum computers alike.

Simulating resonant inelastic x-ray scattering of Ru model complexes using time-dependent density functional theory

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P22

University of Memphis

Resonant inelastic x-ray scattering (RIXS) is an advanced two-photon x-ray spectroscopy technique, where the energy of an incident photon is tuned to coincide with one of the x-ray atomic transitions of the system. RIXS is fast becoming a key instrument to probe the electronic and structural properties of samples in solid, liquid, and gaseous form. This process is theoretically described by the Kramers-Heisenberg equation, which requires the knowledge of excited-state transition moments and energies. Nonetheless, evaluating excited-state transition dipole moments in large transition metal complexes with high-accuracy quantum chemical methods is expensive and oftentimes impractical. In this work, we demonstrate that methods based on time-dependent density functional theory (TD-DFT) can be a valuable alternative for simulating RIXS maps in transition metal complexes. By employing a reduced-cost approach based on the unrelaxed second-order density polarization obtained from linear-response TD-DFT computations, and relativistic effects via the zeroth-order regular approximation (ZORA), we can successfully simulate the 2p3d and 3p4d RIXS maps of Ru model complexes without the need to solve costly quadratic response and relativistic equations. The results illustrate how these methods can be applied to interpret and guide experiments being currently done at state-of-the art light-source facilities, such as LCLS-II.

PolyCrit: An Online Database and Machine Learning Framework for Polymer Characterization by Polymer LCCC

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P23

University of Memphis

Polymer liquid chromatography at critical conditions (LCCC) enables molecular weight independent polymer separation by precisely tuning interactions between stationary and mobile phases. LCCC uniquely facilitates the characterization and separation of complex polymer architectures, including branched, block copolymers, and chemically similar macromolecules, which are challenging to differentiate using conventional chromatographic methods. Despite its advantages, optimizing LCCC conditions is complicated by fragmented literature data and complex interdependencies among experimental parameters. To address these challenges, we have developed PolyCrit, an online database that consolidates 428 experimentally validated polymer critical conditions into a structured, searchable, and publicly accessible platform. Building upon this foundation, we are implementing machine learning models to predict critical conditions for polymers lacking established LCCC conditions. This predictive capability promises to enhance experimental efficiency, accelerate method optimization, and broaden LCCC's accessibility to the polymer science community. This work highlights the creation, features, and current predictive modeling efforts integrated within PolyCrit to advance polymer chromatographic analysis.

Calculation of the Quantum Mechanical Effusion Rate via Miller's Method

Nicholas Corsello*, *Sergei Egorov

P24

University of Virginia

In chemical kinetics, Transition State Theory (TST) is frequently used to approximate thermal rate constants (k(T)) for reactions at a variety of temperatures, however it has been shown to deviate from experimental results if there are significant quantum effects. To adjust for this deviation, many different methods (called quantum TSTs, or QTSTs) have been designed, however none of these methods have yet come forward as universally applicable. The goal of this work is to apply multiple different QTSTs to a hydrogen gas effusion system and compare the rate constant results for the different methods to each other and to the classical results. One such method, developed by William H. Miller showed a decrease in the quantum k(T) from the classical k(T) over the entire studied temperature range and range of effusion gap sizes. An even further decrease was shown when the effusion slit was asymmetric with respect to its wall height in the effusion box. To verify the results, initial investigation has begun into modeling the effusion system with a gaussian wavepacket and obtaining the quantum rate constants via that method.

Implementation of the Gaussian electronic structure program into QCArchive, an open-source ecosystem for large-scale quantum chemistry computations

Dr. Reza Hemmati* and *Dr. Benjamin Pritchard

P25

Virginia Tech

In the era of data generation and analysis, high-quality data is the cornerstone of this realm and computational chemistry is not an exception. One of the ways to obtain chemical data is to employ quantum chemistry computations and extract desired data. These computations can be performed with a desired chemistry software package, but at large-scale, management of the calculations, storage of the results, and retrieval of the results can be a major challenge in creating a dataset. QCArchive, an open source platform for high-throughput computations can handle the situation. At the heart of the QCArchive are the quantum chemistry codes that make those computations possible. To further modular software in QCArchive and to offer new methods and capabilities that allow researchers to study large molecular systems, the Gaussian electronic structure program has been implemented into QCArchive. Therefore, it brings a variety of new methods and enhances the performance of QCArchive project.

Extending Generalized Hybrid Orbitals (GHO) to Model QM/MM Boundaries in Solid Surfaces

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P26

Georgia Tech

Heterogeneous catalysis at solid-liquid interfaces presents a unique opportunity to tune accessible chemistries by modifying the solvent/electrolyte system. Because of the breadth of possible combinations of solid catalyst, solvent composition, and other conditions, computational modeling can serve to identify both promising systems and relevant motifs for performing particular reactions. Modeling reactive processes requires quantum mechanics to resolve the electronic structure, but the number of atoms required to recreate the solid-liquid microenvironment comprising solvent/electrolyte structures and the solid interface prohibits application of ab initio to the full system. Accordingly, we adopt a hybrid quantum mechanical/molecular mechanical (QM/MM) approach to model the electronic structure of the active complex explicitly and represent the remainder of the inert environment with a computationally cheaper forcefield. One challenge presented by this approach is how to handle the boundary created by partitioning the solid surface into QM and MM regions. Common approaches include: link-atom capping schemes, which introduce additional degrees of freedom and require subsequent charge/force redistributions; and solid-state—or effective core potential (ECP)—embedding, which assumes completely ionicity. The generalized hybrid orbital (GHO) method proposed by Gao and co-workers models the boundary between QM and MM regions using local orbitals and maintains charge balance by construction. We present an extension of GHO methodology for modeling boundaries in solid surfaces as well as benchmarks for SiO2.

Speeding Through the Highs and Lows of PNO-CC Response Methods

Jose P. Madriaga* and *Dr. Daniel Crawford

P27

Virginia Tech

The use of natural orbitals (NOs) has revolutionized high-polynomial-scaling coupled-cluster (CC) methods, bringing them closer in efficiency to density functional theory (DFT) while achieving (near) linear scaling for ground-state energetics. In this work, we extend these advances to the calculation of static and electric-field-dependent properties, investigating the benefits and limitations of employing pair natural orbitals (PNOs) within the CC formalism.

Exploring transition metal chemistry using tensor product selected configuration interaction method

Arnab Bachhar*, *Nicholas Mayhall

P28

Virginia Tech

Transition metal complexes present significant challenges for electronic structure methods due to their intricate multireference character and strong electron correlation effects. Traditional wavefunction-based approaches, such as CASSCF, DMRG, etc. can become computationally expensive for large active spaces. We have developed Tensor Product Selected Configuration Interaction (TPSCI) method to exploit the sparse nature of FCI wavefunction by employing selected CI in tensor product basis. TPSCI leverages a tensor product basis constructed from localized molecular orbitals, allowing for an efficient and systematic truncation of the configuration space while maintaining high accuracy. The method involves grouping orbitals into clusters and defining many-particle cluster states within each cluster. Instead of working with Slater determinants, the SCI algorithm is then performed directly in a basis constructed from tensor products of these cluster states. In this work, we demonstrated the applicability of TPSCI to various transition metal systems, analyzing their electronic properties and magnetic interactions mainly focusing on exchange magnetic coupling constant. Benchmark calculations against DMRG reveal that TPSCI provides a balanced trade-off between computational cost and accuracy, making it a promising approach for studying strongly correlated transition metal systems.

Li+ ion transport in high concentration electrolyte (HCE)

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P29

Vanderbilt University

Classical molecular dynamics (cMD) simulations were employed to investigate lithium-ion transport in high-concentration LiFSI/DMC electrolytes. The simulations successfully reproduce the experimentally observed increase in lithium transference number with salt concentration and provide molecular-scale insights into the underlying transport mechanisms. As concentration increases, the solvation structure evolves from a regime dominated by solvent-separated ion pairs (SSIP) and contact ion pairs (CIP) to one dominated by large ion aggregates. This transition correlates with a shift in lithium transport behavior: while vehicular motion dominates at lower concentrations, structural diffusion becomes the primary transport mechanism at higher concentrations. Ion correlation analysis reveals that self-cation conductivity plays a central role in the enhanced transference number, while distinct cation–anion and cation–cation correlations become less influential. Diffusion length analysis shows a shift of transport mechanism from vehicular to structural character, suggesting a shift in character is the key factor enabling efficient lithium transport in highly concentrated LiFSI/DMC electrolytes.

Effect of Numerical Integration Grids in TD-DFT Core-Level Spectra Calculations

Matthew N. Ward*, *Daniel Nascimento

P30

University of Memphis

Time-dependent density functional theory (TD-DFT) is widely used to compute electronic excited state energies due to its cheap cost and reasonable accuracy. Because most TD-DFT methodologies are designed for valence excited states, core-level excitations tend to be significantly underestimated. Nevertheless, with the aid of *a posteriori* shifts, the TD-DFT formalism has been successfully adapted to simulate core-level spectroscopies, such as Resonant Inelastic X-ray Scattering (RIXS). Despite these advancements, routine computations involving transition metal complexes, especially those involving more than a thousand basis functions, are still too expensive for practical purposes. Recent research has shown that the exchange-correlation kernel contributions can be responsible for up to 50% of the computational cost when evaluated on a “moderate” numerical integration grid while having negligible impact on the qualitative aspects of the calculated spectra. In this work, we investigate the implementation of cheaper numerical quadratures and their quantitative contributions in core-level spectroscopy.

Fast simulation of soft x-ray near-edge spectra using a relativistic state-interaction approach: Application to closed-shell transition metal complexes

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P31

University of Memphis

The field of spectroscopy is rapidly advancing, with increasingly sophisticated techniques enabling deeper insights into core-level phenomena. However, accurately simulating these effects—especially at the L- and M-edges—remains a major challenge due to the critical role of spin-orbit coupling. Non-relativistic quantum mechanical methods often fall short, while fully relativistic approaches are computationally prohibitive. In this work, we present a reduced-cost, state-interaction method for simulating near-edge soft X-ray absorption spectra of closed-shell transition metal complexes. Our approach incorporates relativistic effects via the ZORA-Kohn-Sham Hamiltonian and achieves spectral accuracy comparable to more rigorous methods. This makes our method a practical, cost-effective alternative for large-scale simulations and applications.

Completely Renormalized Equation-of-Motion Coupled Cluster in the Exact Two-Component Relativistic Framework

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Florida State University

We have implemented the completely renormalized (CR) triples corrections to excited-state energies obtained using equation-of-motion (EOM) coupled-cluster (CC) theory with singles and doubles (EOMCCSD) that makes use of the exact two-component (X2C) relativistic framework. The resulting CR-EOMCC(2,3) approach improves the underlying X2C-EOMCCSD calculations, as exemplified by analyzing the excitation spectra of the monocations of Cu, Ag, and Au atoms, for which spin–orbit coupling becomes important. Furthermore, the N^7 scaling characterizing the non-iterative CR-EOMCC(2,3) corrections, where N is a measure of the system size, is an order of magnitude smaller than a single iteration of the parent EOMCC approach with up to triples (EOMCCSDT) that scales as N.

The Exact Electron-Photon Exchange-Correlation Potential in Cavity Quantum Electrodynamics Density Functional Theory

Eugene DePrince

P33

Florida State University

The last decade has seen a great deal interest in applications of strong coupling between light and molecular degrees of freedom, the potential applications of which are wide ranging. For the electronic strong coupling problem, cavity quantum electrodynamics (QED) generalizations of many familiar quantum chemistry approaches have been put forward, including a cavity QED form of density functional theory (DFT). As in standard DFT, the exact form of the exchange correlation (XC) functional for QED-DFT is unknown. Here, I will discuss a numerical procedure for extracting the exact electron-photon part of the exchange correlation functional from a procedure based on Levy's constrained search formalism.

Implementation of Ionization-Potential and Electron-Attachment Time-Dependent Equation-of-Motion Coupled-Cluster with Koopman Initial States

P.D. Varuna S. Pathirage, Stephen H. Yuwono, A. Eugene DePrince III

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Florida State University

Here, we present a time-dependent equation-of-motion coupled-cluster (TD-EOM-CC) framework for the simulation open-shell systems through the ionization potential (IP) and electron attachment (EA) EOM-CC formalisms. This formulation of EA-/IP-TD- EOM-CC can use initial state that is defined as 1) the lowest root of an EA-/IP-EOM-CC diagonalization, 2) the lowest root of the 1-particle –1-particle (EA) or 1-hole–1-hole (IP) block of the similarity-transformed Hamiltonian, or 3) the lowest-energy Koopman state. Small systems, including OH radical and Na atom (starting from the closed-shell OH- anion and Na+ cation) were used to test the efficacy of the initial state approximations in recovering the linear absorption spectra of the parent method using the full initial guess.

Analysis of Integrin & CEACAM Expression in Breast Cancer Using GTEx and TCGA data

Urvashi; Hossain Shadman; Xiaohua Huang ; Yongmei Wang

P35

University of Memphis

Integrins and CEACAMs are families of cell adhesion molecules that play crucial role in cell-matrix interactions and are important in cancer development and metastasis. This study analyzed the expression patterns and co-expression relationships of 27 integrin and 12 CEACAM genes in breast tissue using RNA-sequencing data from the GTEx (healthy breast), TCGA (normal), and TCGA (breast cancer) datasets. Gene expression data were retrieved through the UCSC Xena browser platform, and RNA-sequencing datasets were analyzed to investigate the co-expression of integrin and CEACAM genes using Pearson correlation; the top 2000 genes associated with each integrin and CEACAM gene were then selected for further analysis. Functional enrichment using DAVID tool revealed relevant GO Biological process (BP) terms and pathways associated with integrins across the GTEx and TCGA datasets. The results illustrated the overlapping of co-expressed genes across the three datasets. The integrin–CEACAM co-expression networks exhibited both shared and distinct interaction patterns between healthy and cancerous breast tissues, providing valuable insights into the potential roles of these genes in tissue-specific mechanisms of cancer progression and metastasis.

Investigating Interlayer Charge Transport of 2D Hybrid Perovskites via Constrained Density Functional Theory

Jordan Hale, Mikhayla Clothier, Joshua S. Kretchmer

P36

Georgia Tech

The appearance of two-dimensional (2D) layered perovskites has created an exciting overlap of ideas and concepts previously studied separately in 2D heterostructures and 3D bulk perovskites. One feature of stacked 2D heterostructures is the implied mechanistic differences between intralayer (in-plane) and interlayer (out-of-plane) charge transport due to the anisotropic structure. This feature is exemplified in 2D perovskites via the alternating layers of conductive inorganic octahedra and insulative organic spacers, which closely resemble how quantum wells are depicted. Combined with the compositional variety and dynamically disordered nature that perovskites have been known for, there is a wide breadth of physics and potential applications to explore in 2D layered perovskites. Here, in this work, we focus on understanding the behavior of interlayer charge transport in 2D hybrid lead halide perovskites using the constrained density functional theory (cDFT) approach. Assuming a Marcus-like charge transfer picture, cDFT allows us to obtain effective diabatic states that can be used to calculate electronic couplings between the inorganic layers. Using the magnitude of electronic couplings, we can compare the influence of various organic linkers on interlayer charge transfer.

Advancing Homology Modeling: Strategies for Complex Multidomain Fibrous Proteins

Tatyana Denton*, *Sophia Mohamed*, *Katherine Crutchfield*, *Lauren Roberts*, *Emma Wallace*, *Serena D. Stoddard*, *Shana V. Stoddard

P37

Rhodes College

Homology modeling allows scientists to probe structure-function relationships of proteins at the atomic level. The information garnered from homology models can be helpful for the development of biotools and therapeutics, understanding pathological states of diseases, studying protein engineering design, and more. One challenge in homology modeling is the limitation of developing high-quality multidomain models of proteins with fibrous structures and tandem repeats of the same domain type in a contiguous format. In this work a novel approach to developing a multidomain homolog model for the fibrous protein Thrombospondin type-1 containing domain 7A (THSD7A) was evaluated. Models developed using Alpha fold (AF2) and one developed using our novel approach were investigated to determine strengths and strategies for improvement for the next frontier of homology modeling. This work expands on our existing knowledge to introduce strategies and tools to integrate into modeling software to advance our capabilities of accurately developing large, complex, multidomain homology models. Additionally, THSD7A is known to be an antigen in the autoimmune disorder primary membranous nephropathy (PMN). Thus, having an accurate understanding of this protein's structure is vital to development of therapeutic interventions for PMN. Finally, THSD7A is a also member of the thrombospondin repeat (TSR) domain containing super family of proteins, which are known to be heavily involved in binding interactions in the extracellular matrix (ECM) promoting functions such as angiogenesis, cell migration, and tissue remodeling. This work advances our knowledge structure of these proteins which should lead to improvements in understanding how they participate in molecular interactions that influence ECM organization.

Ring strain of cylopropane, cyclobutane, and small heterocycles revisited

David H. Magers

Mississippi College

P38

The strain energy in small cyclic compounds have interested chemists ever since Adolf von Baeyer studied the deviation of normal tetrahedral bond angles in cyclic alkanes in the 1880's. Most studies of ring strain have centered round the strain energy in cyclopropane and cyclobutane. Of course, these systems are the prototypical three- and four-membered rings, but they generate additional interest because of the remarkable similarity of their strain energies, which are almost always reported to lie between 1 and 2 kcal/mol of each other. This result is surprising because cyclopropane must have greater Baeyer or angle strain. The usual explanation is that cyclopropane is stabilized by sigma aromaticity. But cyclopropane is not the only three-membered ring with a relatively small strain energy. The strain of oxirane is quite similar to that of cyclopropane, while the strain of thiirane is much smaller. Yet, the strain energy of silirane is much larger. In the current study, the conventional strain energies of each of these systems is computed with the use of homodesmotic and hyperhomodesmotic models. Natural bond order analysis is employed to help explain the factors contributing to the stabilization of each system.

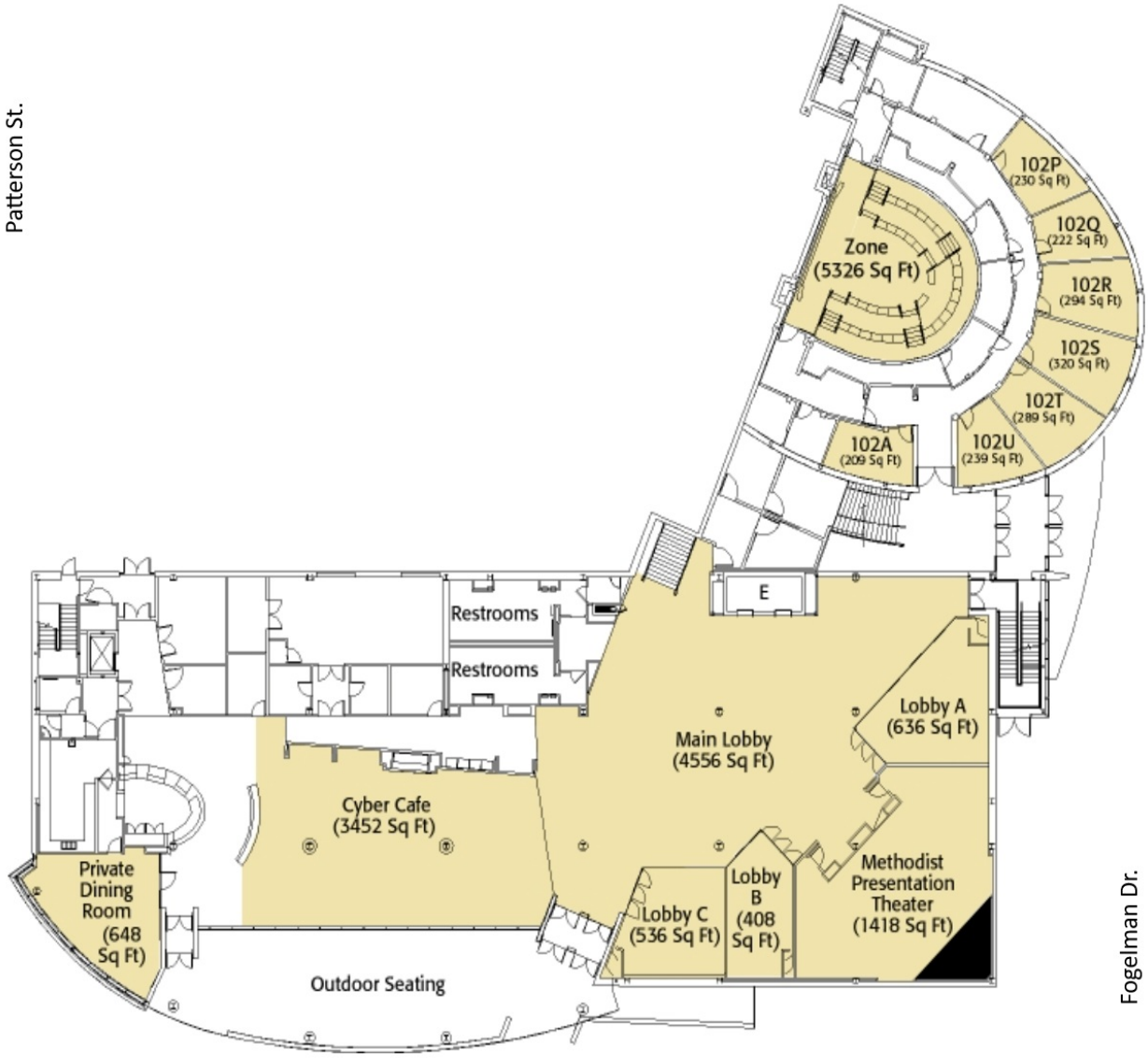
Useful Information

All events will be held at the **FedEx Institute of Technology (FIT)**, 365 Fogelman Drive.

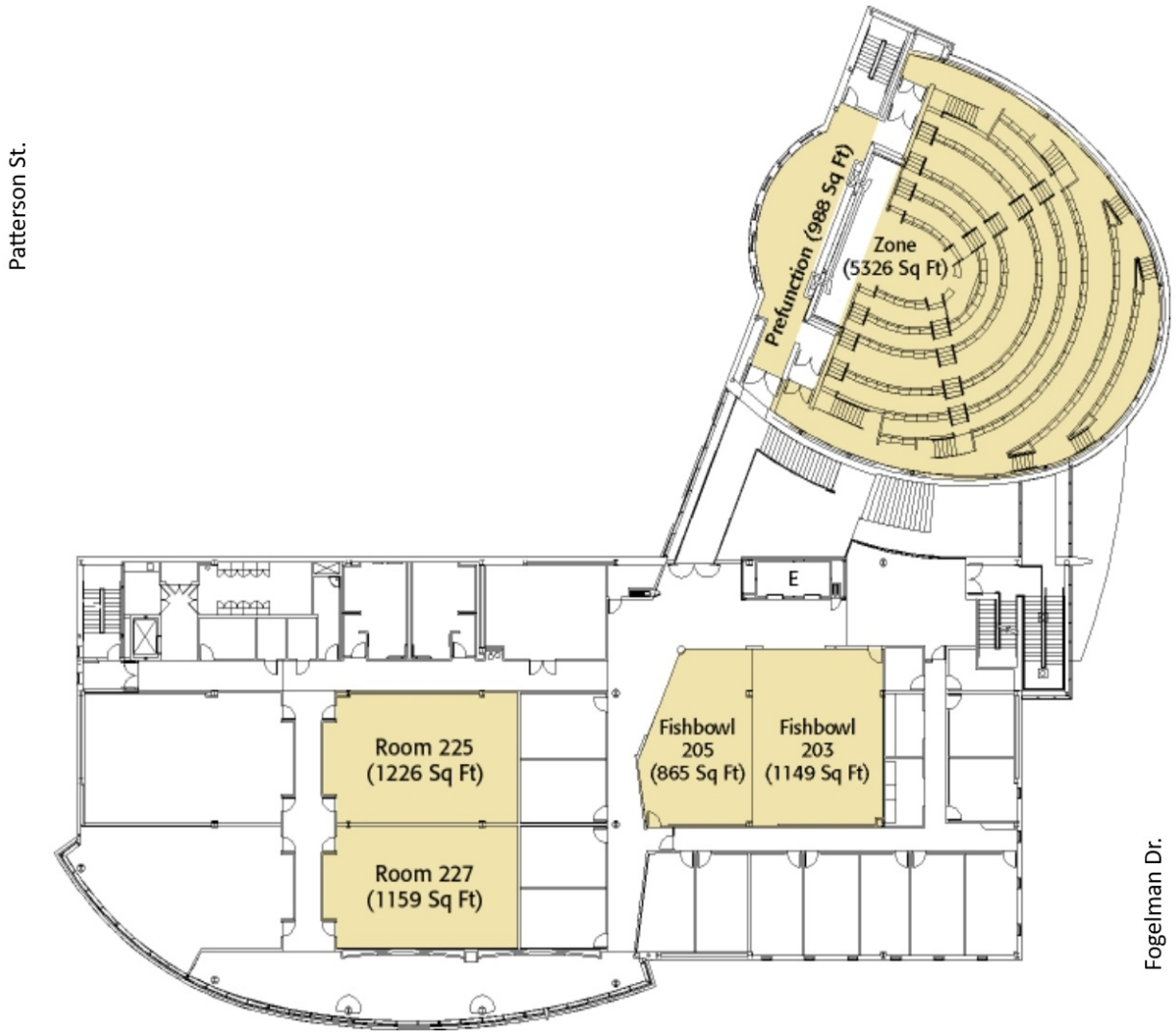
Locations

- **Talks**: *The Zone* (1st floor) – Access via ground floor
- **MolSSI Workshop**: *FishBowl* (2nd floor)
- **Meals/Breaks**: *Main Lobby* (1st floor)
  - Coffee breaks, Thu Welcome Snacks, Fri Lunch & Dinner Reception
- **Posters**: *Cyber Café* (1st floor)
  - Thursday evening & Friday noon
- **Wi-Fi**: UofM Guest Network / eduroam

FIT First Floor

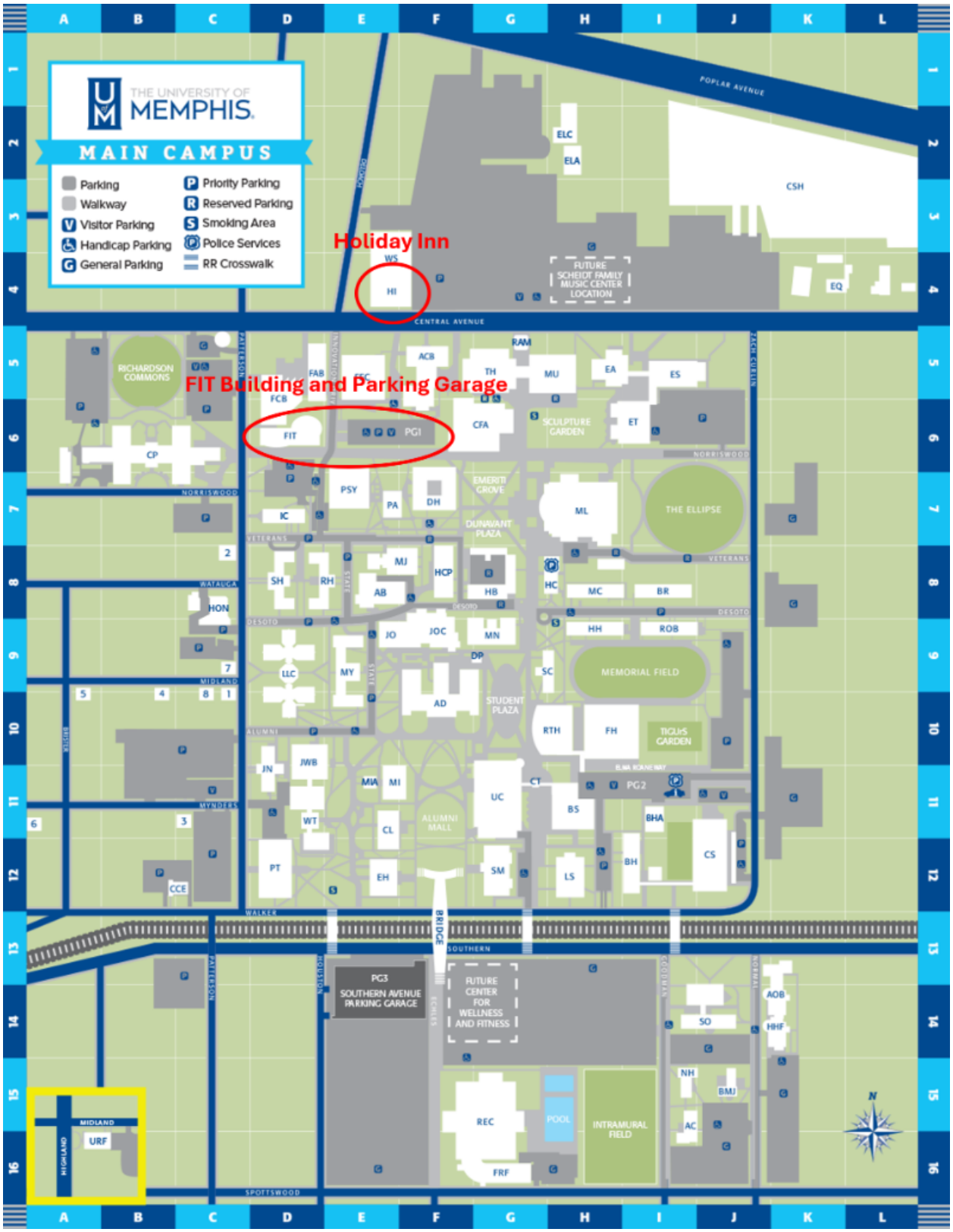


FIT Second Floor



Parking

Visitors can park in the **Fogelman Drive Parking Garage (PGI)**, situated directly across from FIT building.



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Daniel Nascimento (chair)
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