SETCA 2019 Posters

Listed Alphabetically by Presenter’s Last Name

R1) Quasi-degenerate Perturbation Theory for Singlet Fission Bi-exciton States
   *Vibin Abraham* and *Nicholas Mayhall*, Virginia Tech

R2) The Performance of Explicitly Correlated Methods for the Computation of Anharmonic Vibrational Frequencies
   *Donatus Agbaglo* & *Ryan C. Fortenberry*, Georgia Southern University

R3) The proto-Nucleic Acid Builder (pNAB): A Software Tool for Constructing Nucleic Acid Analogs
   *Asem Alenaizan*, *Joshua Barnett*, *Nicholas V. Hud*, *C. David Sherrill*, *Anton S. Petrov*, Georgia Institute of Technology

R4) Probing the O-H and C-H activation for the neutral and charged species of ruthenium mono-oxide species. Ground and excited states calculations
   *Nuno M.S. Almeida*, *Isuru R. Ariyarathna* and *Evangelos Miliordos*, Auburn University

R5) Extending the Aufbau principle of solvated electron precursors to the second solvation shell: The case of M(NH3)4@12NH3 (M=Li, Be+, B2+)
   *Isuru R. Ariyarathna*, *Filip Pawłowski*, *Joseph Vincent Ortiz* and *Evangelos Miliordos*, Auburn University

R6) Electronic and charge-transport properties of donor-acceptor co-crystals
   *Ajith Ashokan*, *Caitlin Hanson*, *Jean-Luc Bredas*, and *Veaceslav Coropceanu*, Georgia Institute of Technology

R7) Application of the Gibbs Phase Rule and Critical Point Universality to Predict Critical Effects in Solid-Liquid Phase Equilibria
   *James K. Baird* and *Xingjian Wang*, University of Alabama in Huntsville

R8) Conformational Energetics of Urea and Thiourea Near the CCSD(T) Complete Basis Set Limit
   *Kayleigh R. Barlow* and *Gregory S. Tschumper*, The University of Mississippi

R47) CrystaLattE: Automated Calculation of Lattice Energies of Organic Crystals
   *Carlos H. Borca*, *Brandon W. Bakr*, *Lori A. Burns*, and *C. David Sherrill*, Georgia Institute of Technology

R9) Characterizing Magnesium Acetylide and its Cation in Silico for Spectroscopic Detection
   *Joseph E. Burns*, *Qianyi Cheng*, *Ryan C. Fortenberry*, *Nathan J. Deyonker*, *The University of Memphis*

R10) Noncovalent Interactions in Networks of Trimethylamine N-oxide, Guanidinium Cation, and Water
    *Mary Hannah Byrd*, *Genevieve Halingten-Verville*, *Nathan I. Hammer*, *Shelley A. Smith*, and *David H. Magers*,
    1Mississippi College 2University of Mississippi

R11) Unraveling the Mechanism of Polyethylene Microstructure Modulation using a Redox-Active Ni-based Olefin Polymerization Catalyst
    *Robert C. Chapleski, Jr.*, *Jesse L. Kem*, *W. Curtis Anderson, Jr.*, *Brian K. Long*, *Sharani Roy*, 1The University of Tennessee, Knoxville, 2Randolph College

R12) Acylation and Deacylation Mechanism and Kinetics of Penicillin G Reaction with Streptomyces R61 DD-peptidase
    *Qianyi Cheng*, *Nathan J. DeYonker*, University of Memphis
R13) In situ Low-temperature Pair Distribution Function (PDF) Analysis and Molecular Dynamics Simulations of CH₄ and CO₂ Hydrates
Bernadette. R. Cladek¹, S. M. Everett², M. T. McDonnell², M. G. Tucker², D. J. Keffer¹, C. J. Rawn¹, ¹University of Tennessee ²Oak Ridge National Laboratory

R14) The Quest for a Local Representation of Virtual Spaces for Embedded Wave Functions
Daniel Claudino and Nicholas J. Mayhall, Virginia Tech

R15) Ab initio investigation of ground states of NbO0
Emily Claveau and Evangelos Miliordos, Auburn University

R16) Lanczos integrators for time-dependent coupled-cluster theory
Brandon C. Cooper and A. Eugene DePrince III, Florida State University

R17) Rovibrational Characterization of [Al,O,C,N] Isomers Using Quartic Force Fields
Megan C. Davis, Tarek Trabelsi, Joseph S. Francisco and Ryan C. Fortenberry, University of Mississippi

Ruhee Dcunha, T. Daniel Crawford, Virginia Tech

R19) Rotational and Vibrational Fingerprints of the Oxywater Cation, a Possible Precursor to Abiotic O₂
Weston Del Rio and Ryan C. Fortenberry, University of Mississippi

R20) Reproducible, Rational, and Rigorous QM-cluster Enzyme Models
Nathan J. DeYonker, Qianyi Cheng, Thomas J. Summers, University of Memphis

R21) Using Dyson orbitals and vertical electron binding energies to predict superacidity in protonated carboranes
Manuel Diaz-Tinoco and J. V. Ortiz, Auburn University

R22) Basin hopping approach to global exploration of self-consistent field solution space
Xinju Dong, University of Louisville

R23) Investigation Into Transition Metal Photocatalytic Materials
Clint Evrard, University of Louisville

R24) Computational Studies of the Interaction between Human Topoisomerase IIα and α-(N)-Heterocyclic Thiosemicarbazones with Molecular Dynamic Simulations
Florence Fabunmi, Tao Yu, Tennessee Technological University

F47) Astrochemistry Made Easy(er) by Quantum Chemistry
Ryan C. Fortenberry, University of Mississippi

Valerie Garcia-Negrón, Akinola D. Oyedele, Eduardo Ponce, Orlando Rios, David P. Harper, and David J. Keffer, University of Tennessee-Knoxville

R26) Spectroscopic Accuracy of Diatomic Molecules with Multiple Quantum Chemistry Programs
Zach L. Glick, Lori A. Burns, C. David Sherrill, Georgia Institute of Technology

R27) Conventional Strain Energies of Thiaphosphirane and the Thiaphosphetanes
Makenzie Griffin, Sarah D. Newell, Shelley A. Smith, and David H. Magers, Mississippi College
R28) Computational Studies on Substrate Binding Motifs in Dissimilatory Sulfite Reductase
Alexa Griffith¹, Ana V. Cunha¹, R. W. A. Havenith², Ashleigh Barnes¹, Dmytro Bykov¹, ¹Oak Ridge National Laboratory, ²University of Groningen

R29) ADAPT Ansatz VQE: Adaptive Derivative-Assembled Pseudo-Trotter
Harper R. Grimsley, Nicholas J. Mayhall, Virginia Tech

R30) Chiral discrimination by intermolecular interaction energies and vibrational spectroscopy in propylene oxide dimers
Reza Hemmati, Konrad Patkowski, Auburn University

R31) Spin-Flip IP/EA: Handling Spin & Spatial Degeneracies With Applications to Double Exchange Systems
Shannon E. Houck, Nicholas J. Mayhall, Virginia Tech

R32) Computational Study of Dehydration and Dehydrogenation of Alcohols on Supported Oxide Catalysis Based on Cyclic (MO2)n (M=Ti, Zr and Hf, n = 2-4) Clusters
Yiqin Hu, Zongtang Fang, Monica Vasiliu, and David A. Dixon, The University of Alabama

R33) Non-Transition-Metal Catalytic System based on Al-Doped Graphene for N2 Reduction to NH3
Yonghui Tian, Shuangli Hu, Xiaolan Sheng, Yixiang Duan, Jacek Jakowski, Bobby G. Sumpter, Jingsong Huang, Oak Ridge National Laboratory

R34) Quantum chemistry on quantum computer: benchmark, unitary-mapped imaginary time evolution
Renke Huang, Francesco A. Evangelista, Emory University

R35) A computational study of CO2 interactions with functionalized calixarene molecules
John H. Hymel, Jacob Townsend, Konstantinos D. Vogiatzis, University of Tennessee

R36) Elucidation of the Reaction Mechanism of C2+N1 Aziridination from Tetracarbene Iron Catalysts
Sara Isbill, Preeti Chandrachud, Jesse Kern, David Jenkins, Sharani Roy, University of Tennessee, Knoxville

R37) Quantum chemistry benchmark for near time quantum computing
Jacek Jakowski, Alex McCaskey, Zach Parks, Shirley Moore, Raphael Pooser, Travis Humble, Oak Ridge National Laboratory

R38) Ab initio investigation of ground and excited electronic states of ZrO
Benjamin Jackson, Evangelos Miliordos, Auburn University

R39) Intrinsic Energetics of Proton Transfer in Concentrated Binary (HCl)m(H2O)n Clusters
Sarah N. Johnson and Gregory S. Tschumper, University of Mississippi

R40) Computational Studies of Neutral and Cationic (UO3)n Clusters: Cluster Formation and Decomposition
Paula Kahn, Monica Vasiliu, David A Dixon, University of Alabama

R41) Oriented Electric Fields Selectively Control the Multistate Reaction Pathways in Azobenzene
Emily M. Kempfer and Lee M. Thompson, University of Louisville

R42) Comparison of full-DFT and semiempirical tight-binding methods in modeling the branching pathway of a Ni-diimine polyethylene catalyst
Jeffrey A. Laub and Jesse L. Kern, Randolph College

R43) Theoretical study of a complete catalytic cycle for methane to methanol transformation facilitated by metal methoxides
Shahriar N Khan, Evangelos Miliordos, Auburn University

SETCA 2019. R: Thursday Poster Session; F: Friday Poster Session
R44) Electronic Structure of Diatomic 3d-Transition Metal Oxides and the Effects of Ligand Field
Introduction
Justin Kyle Kirkland and Konstantinos D. Vogiatzis, University of Tennessee, Knoxville

R45) Modeling of Structural Features in Lignin Based Composite Materials by Hierarchical
Decomposition of the Radial Distribution Function
Dayton G. Kizzire, Valerie García Negrón, David P. Harper, David J. Keffer

R46) Explicitly correlated dispersion and exchange dispersion energies in symmetry-adapted
perturbation theory
Monika Kodrycka and Konrad Patkowski, Auburn University

F1) Modeling the Formation of Atmospheric S-Based Brønsted Acid Gases and their Degradation
Effects on MOF-2 Nanoclusters
Zachary Lee, Shengjie Zhang, Luis Flores and David A. Dixon, The University of Alabama

F2) Mechanisms of Mobile Ion Hopping in Polymerized Ionic liquids
Xubo Luo, Hongjun Liu, and Stephen J. Paddison, The University of Tennessee

F3) Open-Source Numerical Tensor Algebra Library for Heterogeneous Computing in Quantum Many-
Body Theory
Dmitry I. Lyakh, Oak Ridge National Laboratory

F4) A variational approach for the calculation of excited states
Andrew Mahler, Lee M. Thompson, University of Louisville

F5) A dynamical correlation model for variational two-electron reduced density matrix driven complete
active space self-consistent field methods.
Elvis Maradzike, A. E. DePrince, III, Florida State University

F6) Computational studies of alkanol reaction pathways on a SrTiO$_3$ perovskite surface
K. Reid Mason, Robert C. Chapleski Jr., and Sharani Roy, The University of Tennessee, Knoxville

F7) Uncovering f-Block Element Separations Pathways Through Computational Methods
Marcos Mason, Caris Smith, Monica Vasiliu, David A. Dixon, University of Alabama

F8) Selecting Basis Sets, Density Functionals, and Relativistic Corrections for Computations of
Lanthanide-Containing Molecules
Gavin A. McCarver, Robert J. Hinde, Konstantinos D. Vogiatzis, University of Tennessee, Knoxville

F9) Approaches for Machine Learning of Ab Initio Intermolecular Properties
Derek P. Metcalf, Daniel Nascimento, Alexios Koutsoukas, Steven Spronk, Daniel Cheney, C. David Sherrill,
Georgia Institute of Technology

F10) TDDFT Modeling of TiO2 Using Bulk-Mimicking Finite Clusters
Alexander Matthew Meyer, Pragathi Darapaneni, James Dorman and Kenneth Lopata, Louisiana State University

F11) Describing Atomic Oxygen Interactions with Ag(110) Using a Site-Specific Adsorption Model
Carson Mize, Sara Isbill, and Sharani Roy, University of Tennessee, Knoxville

F12) Unique error metric and lower-bound in Kohn-Sham Density Functional Theory
Mohammad Mostafanejad and Albert Eugene DePrince III, Florida State University

F13) Conventional Strain Energies of Thiirane, Thietane, Borylthiirane, 2-Borylthietane, and 3-
Borylthietane
Summer L. Nash, Mary Morgan Mohamed, Shelley A. Smith, and David H. Magers, Mississippi College

SETCA 2019. R: Thursday Poster Session; F: Friday Poster Session
F14) Computational analysis of lamin A structure and dynamics
*Acacia Nicholson, Quentin Johnson, Berry College*

F15) Density Fitting in Exoscale Applications
*Joseph Senan O’Brien and C. David Sherrill, Georgia Institute of Technology*

(abstract withdrawn) Examining properties of Catechol-O-methyltrasnferase while systematically increasing QM-cluster model size.
*Manuel A. Palma, Thomas Summers, Qianyi Cheng and Nathan. J. DeYonker, University of Memphis*

F17) Gas Phase Spectra of MgF2 and MgH2 Molecules and their Dimers: A Possible Connection from Gas-Phase Molecules to Planet Formation
*C. Zach Palmer and Dr. Ryan C. Fortenberry, Georgia Southern University*

F18) Confinement Effects on Electrostatic Screening, Structure, and Dynamics of Ionic Liquids
*Suehyun Park, Yi-Jung Tu, Jesse McDaniel, Georgia Institute of Technology*

F19) Performances of QTP functionals for the excited state energies
*Young Choon Park, Ajith Perera, and Rodney J. Bartlett, University of Florida*

F20) Conformational Analysis of Pi-Conjugated Organic Oligomers
*Morgan A. Perkins, Thomas L. Ellington and Gregory S. Tschumper, University of Mississippi*

F21) Basis Set Superposition Errors in the Many-Body Expansion of Molecular Properties
*Benjamin G. Peyton, T. Daniel Crawford, Virginia Tech*

F22) Benchmark interaction energy studies on the S66 and S66x8 datasets using explicitly correlated approaches with bond functions
*Ian Pimienta and Konrad Patkowski, Auburn University*

F23) Molecular modeling of methane transport in silicate frameworks
*Hadi Rahmani, Tom Pace and Peter Kekenes-Huskey, University of Kentucky*

F16) Approximate Spin-adapted Treatment of Single Reference Coupled Cluster for Open-shell Molecules
*Moneesha Ravi, Ajith Perera, Rodney J. Bartlett, University of Florida*

F24) How Do Amine Bridges Affect Conjugation in Monomacrocyclic Dendrimer Models?
*R. Shelby Ruiz, Aubrey Smyly, Trent Selby, David H. Magers, and Shelley A. Smith, Mississippi College*

F25) The Rovibrational Characteristics of Ammonia Borane
*Spencer C. Rushing, Ryan C. Fortenberry, and Gregory S. Tschumper, University of Mississippi*

F26) Electronically Excited States of Closed-Shell, Functionalized Benzene (-CN, -OH, -C2H) Anions
*Taylor Santalocci and Ryan Fortenberry, University of Mississippi*

F27) Geometries, Energetics and Harmonic Vibrational Frequencies of Structurally Diverse Hydrated Halide ions by the 2-body: Many-body Method
*Thomas More Sexton, Caroline Anne Rader and Gregory S. Tschumper, University of Mississippi*

F28) Direct Entropy Calculation from Molecular Dynamics Simulation
F29) Intramolecular Hydrogen Bonding in Epoxide, Thiirane, Aziridine and Phosphirane Containing Cyclopentanols  
*Ben E. Smith*, Jeremy M. Carr and Gregory S. Tschumper, 1University of Mississippi, 2Central Alabama Community College

F30) DAT 30: Dative Bonding Benchmark Database  
*Brett Smith, Konstantinos Vogiatzis*, The University of Tennessee Knoxville

F31) Multiscale Modeling of a Functionalized Surface Catalyst for Hydrogen Peroxide Production  
*Yuny Snyder*, Randolph College

F32) Quantifying Protein Contact Networks through Residue-Residue Pair Interaction Energies  
*Thomas J. Summers, Baty Daniel, Qianyi Cheng, and Nathan J. DeYonker*, University of Memphis

F33) Data-driven Acceleration of the Coupled-cluster Eigensolver  
*Jacob Townsend and Konstantinos Vogiatzis*, University of Tennessee

F34) Characterization of inner-layer capacitance from constant voltage molecular dynamics  
*Yi-Jung Tu, Sam Delmerico, Jesse G. McDaniel*, Georgia Institute of Technology

F35) Spinel Nanocrystals for Insights into Planet Formation  
*E. Michael Valencia, Ryan C. Fortenberry*, University of Mississippi

F36) An adiabatic connection formalism for doubly-occupied configuration wavefunctions as a new approach to capture dynamical correlation in strongly correlated systems  
*Nam Vu*, Florida State University

F37) Spin splittings from first-order symmetry-adapted perturbation theory without the single exchange approximation  
*Jonathan Waldrop and Konrad Patkowski*, Auburn University

F38) Electron correlation in chemical bonds II. LiH and LiH+  
*Shehani T. Wetthasinghe, Vitaly A. Rassolov*, University of South Carolina

F39) Coordination Modes of Nitrogen to Molybdenum: An ab initio Electronic Structure Study  
*Maria V. White, Justin K. Kirkland, Konstantinos Vogiatzis*, University of Tennessee

F40) Nuclear wavefunction dynamics with trajectory guided fully adaptable gaussian bases  
*Sachith Wickramasinghe, Sophya Garashchuk*, University of South Carolina

F41) Versatility of the QTP family of DFT functionals: Predicting Fermi contact and extended system’s band gap  
*Zachary W. Windom, Ajith Perera, Rodney Bartlett*, University of Florida

F42) The Shapes of the Smallest Rocks  
*Charlie Worth, Ryan C. Fortenberry*, University of Mississippi

F43) Efficient Implementation of Density Functional Theory Based Symmetric Adapted Perturbation Theory  
*Yi Xie, Daniel G. A. Smith and C. David Sherrill*, Georgia Institute of Technology

F44) Calculation of Accurate Low Intensity Strong Field Ionization Rate  
*Mengqi Yang, Kenneth Lopata*, Louisiana State University

F45) Apply Machine Learning Models in Predicting Magnetic Moment of Ferrite Material  
*Jiazhou Zhu, Rachel Getman*, Clemson University

SETCA 2019. R: Thursday Poster Session; F: Friday Poster Session
F46) Proton Dissociation and Transfer in Protic Ionic Liquids (PILs)
Zhenghao Zhu, Xubo Luo, and Stephen J. Paddison, University of Tennessee, Knoxville