

# SETCA 2019 Posters

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### **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(NH<sub>3</sub>)<sub>4</sub>@12NH<sub>3</sub> (M=Li, Be<sup>+</sup>, B<sub>2</sub><sup>+</sup>)**

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<sup>1</sup>, Genevieve Halingten-Verville<sup>2</sup>, Nathan I. Hammer<sup>2</sup>, Shelley A. Smith<sup>1</sup>, and David H. Magers<sup>1</sup>,

<sup>1</sup>Mississippi College <sup>2</sup>University of Mississippi

### **R11) Unraveling the Mechanism of Polyethylene Microstructure Modulation using a Redox-Active Ni-based Olefin Polymerization Catalyst**

Robert C. Chapleski, Jr.<sup>1</sup>, Jesse L. Kern<sup>2</sup>, W. Curtis Anderson, Jr.<sup>1</sup>, Brian K. Long<sup>1</sup>, Sharani Roy<sup>1</sup>, <sup>1</sup>The University of Tennessee, Knoxville, <sup>2</sup>Randolph College

### **R12) Acylation and Deacylation Mechanism and Kinetics of Penicillin G Reaction with Streptomyces**

#### **R61 DD-peptidase**

Qianyi Cheng, Nathan J. De Yonker, University of Memphis

**R13) In situ Low-temperature Pair Distribution Function (PDF) Analysis and Molecular Dynamics Simulations of CH<sub>4</sub> and CO<sub>2</sub> Hydrates**

Bernadette R. Cladek<sup>1</sup>, S. M. Everett<sup>2</sup>, M. T. McDonnell<sup>2</sup>, M. G. Tucker<sup>2</sup>, D. J. Keffer<sup>1</sup>, C. J. Rawn<sup>1</sup>, <sup>1</sup>University of Tennessee <sup>2</sup>Oak 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

**R18) Can Density-Functional Theory Simulate Complex Solvent Effects? A Study of Chiral Imprinting Using Molecular Dynamics and Quantum Chemistry**

Ruheen Dcunha, T. Daniel Crawford, Virginia Tech

**R19) Rotational and Vibrational Fingerprints of the Oxywater Cation, a Possible Precursor to Abiotic O<sub>2</sub>**

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

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Florence Fabunmi, Tao Yu, Tennessee Technological University

**F47) Astrochemistry Made Easy(er) by Quantum Chemistry**

Ryan C. Fortenberry, University of Mississippi

**R25) An Efficient Physics-based Model of Structural Features in Composite Materials by Hierarchical Decomposition of the Radial Distribution Function**

Valerie García-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 Griffing, Sarah D. Newell, Shelley A. Smith, and David H. Magers, Mississippi College

**R28) Computational Studies on Substrate Binding Motifs in Dissimilatory Sulfite Reductase**  
Alexa Griffith<sup>1</sup>, Ana V. Cunha<sup>1</sup>, R. W. A. Havenith<sup>2</sup>, Ashleigh Barnes<sup>1</sup>, Dmytro Bykov<sup>1</sup>, <sup>1</sup>Oak Ridge National Laboratory, <sup>2</sup>University 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 (MO<sub>2</sub>)<sub>n</sub> (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 AI-Doped Graphene for N<sub>2</sub> Reduction to NH<sub>3</sub>**  
Yonghui Tian, Shuangli Hu, Xiaolan Sheng, Yixiang Duan, Jacek Jakowski, Bobby G. Sumpter, Jingsong Huang, Oak Ridge National Laboratory

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Renke Huang, Francesco A. Evangelista, Emory University

**R35) A computational study of CO<sub>2</sub> interactions with functionalized calixarene molecules**  
John H. Hymel, Jacob Townsend, Konstantinos D. Vogiatzis, University of Tennessee

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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)<sub>m</sub>(H<sub>2</sub>O)<sub>n</sub> Clusters**  
Sarah N. Johnson and Gregory S. Tschumper, University of Mississippi

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Paula Kahn, Monica Vasiliu, David A Dixon, University of Alabama

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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

**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<sub>3</sub> 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

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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

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Alexander Matthew Meyer, Pragathi Darapaneni, James Dorman and Kenneth Lopata, Louisiana State University

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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

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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-methyltransferase 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 MgF<sub>2</sub> and MgH<sub>2</sub> 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

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Suehyun Park, Yi-Jung Tu, Jesse McDaniel, Georgia Institute of Technology

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Young Choon Park, Ajith Perera, and Rodney J. Bartlett, University of Florida

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Morgan A. Perkins, Thomas L. Ellington and Gregory S. Tschumper, University of Mississippi

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Benjamin G. Peyton, T. Daniel Crawford, Virginia Tech

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Ian Pimienta and Konrad Patkowski, Auburn University

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Hadi Rahmani, Tom Pace and Peter Kekenes-Huskey, University of Kentucky

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Moneesha Ravi, Ajith Perera, Rodney J. Bartlett, University of Florida

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R. Shelby Ruiz, Aubrey Smyly, Trent Selby, David H. Magers, and Shelley A. Smith, Mississippi College

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Spencer C. Rushing, Ryan C. Fortenberry, and Gregory S. Tschumper, University of Mississippi

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Taylor Santaloci 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**

Clifton C. Sluss, D.M. Nicholson, C.Y. Gao, M.T. McDonnell, D.J. Keffer, University of Tennessee Knoxville

**F29) Intramolecular Hydrogen Bonding in Epoxide, Thiirane, Aziridine and Phosphirane Containing Cyclopentanols**

Ben E. Smith<sup>1</sup>, Jeremy M. Carr<sup>2</sup> and Gregory S. Tschumper<sup>1</sup>, <sup>1</sup>University of Mississippi, <sup>2</sup>Central 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**

Yuriy Snyder, Randolph College

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Thomas J. Summers, Baty Daniel, Qianyi Cheng, and Nathan J. DeYonker, University of Memphis

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Jacob Townsend and Konstantinos Vogiatzis, University of Tennessee

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Yi-Jung Tu, Sam Delmerico, Jesse G. McDaniel, Georgia Institute of Technology

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E. Michael Valencia, Ryan C. Fortenberry, University of Mississippi

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Nam Vu, Florida State University

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Jonathan Waldrop and Konrad Patkowski, Auburn University

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Shehani T. Wetthasinghe, Vitaly A. Rassolov, University of South Carolina

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Maria V. White, Justin K. Kirkland, Konstantinos Vogiatzis, University of Tennessee

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Sachith Wickramasinge, Sophya Garashchuk, University of South Carolina

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Charlie Worth, Ryan C. Fortenberry, University of Mississippi

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Mengqi Yang, Kenneth Lopata, Louisiana State University

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Jiazhou Zhu, Rachel Getman, Clemson University

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Zhenghao Zhu, Xubo Luo, and Stephen J. Paddison, University of Tennessee, Knoxville