

# SETCA 2019 Posters: Friday (F)

## Listed by Poster Assignment

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### **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

### **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 TiO<sub>2</sub> 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

### **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

**F16) Approximate Spin-adapted Treatment of Single Reference Coupled Cluster for Open-shell Molecules**

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

**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

**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

**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, -C<sub>2</sub>H) Anions**

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

**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

**F46) Proton Dissociation and Transfer in Protic Ionic Liquids (PILs)**

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

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

Ryan C. Fortenberry, University of Mississippi