

SETCA 2017

Organizers:

Gregory S. Tschumper – University of Mississippi

Nathan J. DeYonker – University of Memphis

Sponsors:



University of Mississippi

College of Liberal Arts

Office of Research and Sponsored Programs

Department of Chemistry and Biochemistry

MCSR



University of Memphis

College of Arts and Sciences

Department of Chemistry

CROMIUM

Campus Wide Internet

Name: eduroam
Password: institutional
login info
(if your univ. participates)

Coulter Hall Internet

Name: Coulter322A
Coulter322-5G
Password: setca2017

Ford Ballroom Internet

Name: Guest
Password: gorebs

Additional information including parking, conference venues, and lunch locations available on the website:

http://quantum.chem.olemiss.edu/SETCA_2017/

Feedback is welcomed, please email setca2017@olemiss.edu

Friday Morning Session – Coulter Hall Room 211

Chair: Gregory S. Tschumper

Registration	7:15 AM – 10:00 AM
Opening Remarks	8:00 AM – 8:10 AM
IL1 – <u>A. Eugene DePrince, III</u> Quantum Chemistry without Wavefunctions	8:10 AM – 8:40 AM
CL1 – <u>Daniel Claudino</u> New primitive Gaussians based on per electron energy convergence criteria	8:40 AM – 9:00 AM
IL2 – <u>Steven E. Wheeler</u> Tools for the Computational Design of Asymmetric Catalysts	9:00 AM – 9:30 AM
Coffee Break – Snacks and Refreshments Provided	9:30 AM – 9:50 AM
IL3 – <u>Francesco A. Evangelista</u> Electron correlation methods for near-degenerate electronic states based on the driven similarity renormalization group	9:50 AM – 10:20 AM
CL2 – <u>Dominic A. Sirianni</u> Psi4NumPy: An Interactive Quantum Chemistry Programming Environment for Reference Implementation, Rapid Development, and Education	10:20 AM – 10:40 AM
IL4 – <u>T. Daniel Crawford</u> The Molecular Science Software Institute	10:40 AM – 11:10 AM
Lunch – On Your Own Afternoon session starts at 1:00 PM	11:20 AM – 1:00 PM

Friday Afternoon Session – Coulter Hall Room 211

Chair: T. Daniel Crawford

IL5 – David A. Dixon 1:00 PM – 1:30 PM
Interactions of CO₂ with metal organic frameworks and metal oxide nanoclusters

CL3 – Sara Isbill 1:30 PM – 1:50 PM
Interaction of Atomic Oxygen with Ag(111) and Ag(110) Surfaces: Oxygen Adsorption and Kinetics at Surface versus Subsurface

IL6 – Elena Jakubikova 1:50 PM – 2:20 PM
Two-step model of ultrafast interfacial electron transfer in dye-semiconductor assemblies

Coffee Break – Snacks and Refreshments Provided 2:20 PM – 2:40 PM

IL7 – Charles Edwin Webster 2:40 PM – 3:10 PM
Theoretical studies of phosphoryl transfer enzymes

CL4 – Carlos H. Borca 3:10 PM – 3:30 PM
CAM-LDA0: The Reincarnation of the Local Density Approximation

IL8 – Shelley A. Smith 3:30 PM – 4:00 PM
Why Computational Chemists Should Not Be Ignored: The Effect of Ether and Amine Bridges in the Conjugation of Monomacrocyclic Dendrimers

IL9 – John F. Stanton 4:00 PM – 4:30 PM
Thermochemistry: Not as Boring as You Might Think

Friday Evening Session – Inn at Ole Miss: Ford Ballroom

Poster Session – Chair: Nathan J. DeYonker 5:15 PM – 7:15 PM

Banquet – Speaker: Elfi Kraka 7:00 PM – 9:00 PM

Saturday Morning Session – Coulter Hall Room 211

Chair: Nathan J. DeYonker

Doors Open	7:30 AM
IL10 – <u>Evangelos Miliordos</u> An economical theory for chemical bonding	8:00 AM – 8:30 AM
CL5 – <u>J. Coleman Howard</u> Excited State Transition Energies and Properties in Solution from a Smooth Dielectric Model	8:30 AM – 8:50 AM
CL6 – <u>Qianyi Cheng</u> Folding Mechanisms of Small Proteins GB1 and LB1	8:50 AM – 9:10 AM
IL11 – <u>Elfi Kraka</u> A Direct Measure of Metal-Ligand Bonding Replacing the Tolman Electronic Parameter	9:10 AM – 9:40 AM
Coffee Break – Snacks and Refreshments Provided	9:40 AM – 10:00 AM
IL12 – <u>Jing Kong</u> Density Functional Theory Method for Nondynamic/Strong Correlation	10:00 AM – 10:30 AM
CL7 – <u>Thomas Sommerfeld</u> Resonance Energies and Lifetimes from Extrapolation Methods: Robust Algorithms and a Critical Analysis	10:30 AM – 10:50 AM
CL8 – <u>Ryan C. Fortenberry</u> Can We Find Interstellar Nitrogen in Exotic Molecules?	10:50 AM – 11:10 AM
IL13 – <u>Joel Bowman</u> Proton-Bound Complexes: A Major Challenge for Vibrational Analysis	11:10 AM – 11:40 AM
IL14 – <u>Kenneth Lopata</u> Core-Hole Initiated Charge Migration with TDDFT	11:40 AM – 12:10 PM
Business Meeting	12:10 PM – 12:30 PM
Meeting Adjourns	12:30 PM