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 – A. Eugene DePrince, III
Quantum Chemistry without Wavefunctions
8:10 AM – 8:40 AM

CL1 – Daniel Claudino
New primitive Gaussians based on per electron energy convergence criteria
8:40 AM – 9:00 AM

IL2 – Steven E. Wheeler
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 – Francesco A. Evangelista
Electron correlation methods for near-degenerate electronic states based on the driven similarity renormalization group
9:50 AM – 10:20 AM

CL2 – Dominic A. Sirianni
Psi4NumPy: An Interactive Quantum Chemistry Programming Environment for Reference Implementation, Rapid Development, and Education
10:20 AM – 10:40 AM

IL4 – T. Daniel Crawford
The Molecular Science Software Institute
10:40 AM – 11:10 AM

Lunch – On Your Own
11:20 AM – 1:00 PM
Afternoon session starts at 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

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