Southeastern Theoretical Chemistry Association Meeting

2018

Louisiana State University,
Center for Computation and Technology

May 18-19, 2018

Organizer: Kenneth Lopata, Louisiana State University
Department of Chemistry, Center for Computation and Technology

Additional information available at: https://www.cct.lsu.edu/SETCA

Friday May 18, 2018

8:00 AM	**-**	**8:30 AM**	**Registration**	**Digital Media Center (DMC) Lobby**	
8:30 AM	**-**	**10:00 AM**	**Session A**	**DMC Theater**	
		IL1	Greg Tschumper	University of Mississippi	Big Electronic Structure Computations for Small Hydrated Anions
		IL2	Nathan DeYonker	University of Memphis	Inorganic Computational Astrochemistry: Rovibrational Spectroscopy and Heterogenous Catalysis
		CL1	Caitlin Bresnahan	Louisiana State University	A Reactive Empirical Force-Field for HCl Water Clusters
10:00 AM	**-**	**10:15 AM**	**Coffee Break**	**DMC Lobby**	
10:15 AM	**-**	**11:30 AM**	**Session B**	**DMC Theater**	
		IL3	Ye Xu	Louisiana State University	Electric field effects on the stability of molecular superoxide intermediates in non-aqueous oxygen reduction reaction
		CL2	Young Choon Park	University of Florida	Absorption spectrum calculations from the time-dependent EOM-CC theory
		CL2	Elvis Maradzike	Florida State University	Simulation of X-ray absorption spectra using variationally optimized reduced-density matrices within the extended random phase approximation
11:30 AM	**-**	**1:30 PM**	**Lunch**	**On your own**	
1:30 PM	**-**	**3:00 PM**	**Session C**	**DMC Theater**	
		IL4	Jianwei Sun	Tulane University	The Strongly Constrained and Appropriately Normed Meta-Generalized Gradient Approximation
		IL5	Jing Kong	Middle Tennessee State University	Computation of Nondynamic Correlation with Density Functional Theory
		CL4	Duminda Ranasinghe	University of Florida	Accurate description of band gaps in conjugated polymers with CAMQTP functionals
3:00 PM	**-**	**3:15 PM**	**Coffee Break**	**DMC Theater**	
3:15 PM	**-**	**4:30 PM**	**Session D**	**DMC Theater**	
		IL6	Evangelos Miliordos	Auburn	Metal-ammonia complexes disclose a secret

				University	periodic table of solvated electron precursors
		CL5	Nuno Almeida	Auburn University	Novel Transition Metal Chemistry Applied to Solvated Electron Precursors
		CL6	Thomas Summerfeld	Southeastern Louisiana University	Ring-Opening Attachment as an Explanation for the Long Lifetime of the Perfluorotetrahydrofuran Anion
4:30 PM	**-**	**6:30 PM**	**Poster Session**	**DMC Lobby**	
7:00 PM	**-**	**9:00 PM**	**Dinner**	**Andonie Museum at Lod Cook**	
			Keynote Speaker: Bin Chen, Lousiana State University		

Saturday May 19, 2018

8:30 AM	**-**	**10:00 AM**	**Session E**	**DMC Theater**	
		IL7	David Sherril	Georgia Tech	Applications of Partitioned Symmetry-Adapted Perturbation Theory to Drug Binding and Organocatalysis
		CL8	Lori Burns	Georgia Tech	Enhancements and Interoperability in Psi4
		IL8	Eugene DePrince	Florida State University	Dynamical correlation models for variational two-electron reduced-density-matrix driven complete active space self-consistent field methods
10:00 AM	**-**	**10:15 AM**	**Coffee Break**	**DMC Lobby**	
10:15 AM	**-**	**12:00 PM**	**Session F**	**DMC Theater**	
		CL8	Jim Baird	University of Alabama, Huntsville	Anomalous Solubility of Solids in Binary Liquid Mixtures with a Consolute Point
		CL9	Aliasghar Sepehri	Louisiana State University	A Jacobian-Gaussian Method for Efficient Exploration of Conformational Space
		CL10	Sara Isbill	The University of Tennessee, Knoxville	Interaction of Atomic Oxygen with the Ag(111) Surface: Oxygen Adsorption and Kinetics at Surface versus Subsurface
		IL9	Konstantinos Vogiatzis	The University of Tennessee, Knoxville	Evaluation of Catalytic Descriptors with Strongly Correlated Methods and Machine Learning
12:00 PM	**-**	**12:30 PM**	**Business Meeting**	**DMC Theater**	
12:30 PM			**Meeting Ends**		

Poster Presentations
Friday May 18, 4:30 PM - 6:30 PM
Digital Media Center

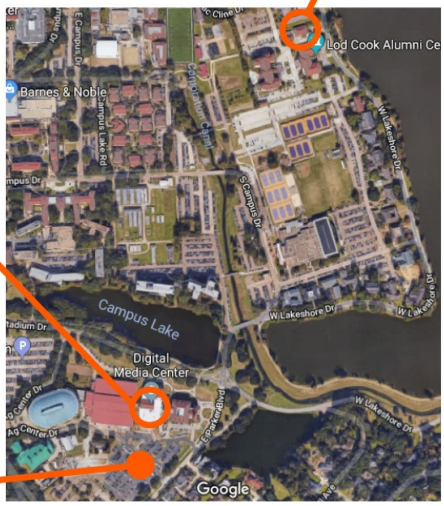
Adonay Sissay	Louisiana State University	Angle-Dependent Strong-Field Molecular Ionization Yields with Tuned Range-Separated Time-Dependent Density Functional Theory
Asim Alenaizan	Georgia Tech	Self-Assembly of Nucleobases Analogues: Quantum Mechanical and Molecular Dynamics Study
Caitlin Bresnahan	Louisiana State University	Developing Reactive Force-Fields for Water Clusters Containing HCl
Chuanlin Zhao	Louisiana State University	Mechanistic Study on C-C Coupling of Acetaldehyde on Partially Reduced CeO2-x(111)
Dominic Sirianni	Georgia Tech	Assessment of Density Functional Methods for Geometry Optimization of Bimolecular van der Waals Complexes
Fenner Colson	Santa Fe College	Anomalous Knudsen Diffusion in Silicate Membranes
Hailey Reed	University of Mississippi	Energetics and vibrational signatures of argyrophilic interactions involving high energy density materials
Ian Pimienta	Auburn University	The molecular structures of 1,1’-Azobis(tetrazole) (N10) and monosubstituted compounds
Isuru Ariyarathna	Auburn University	Aufbau Rules for Solvated electron precursors: The case of super atomic Mg(NH3)40
Jonathan Waldrop	Auburn University	Models of Metal-Organic Frameworks and their interactions with CO2
Justin Kirkland	University of Tennessee, Knoxville	Ligand field effects on the reaction channels of non-heme Fe(IV)-oxos for C-H activation
Ke Li	Louisiana State University	Investigation of Structure and Dynamics of Glyme Based Electrolytes for Sodium Rechargeable Batteries
Matthew Wang	Middle Tennessee State University	Performance of Some of the Latest Density Functional Methods
Moneesha Ravi	Florida State University	Isomerization and Dissociation of Acetylene Di-cation
Monika Kodrycka	Auburn University	Deducing the Optimal Damping Function for the D3 Dispersion Correction to Density Functional Theory
Noor Md Shahriar Khan	Auburn University	Superatomic nature of Sc(NH3)60,+: one and two electrons bound to the periphery of Sc(NH3)62+ core
Paul Abanador	Louisiana State University	Wavelength and intensity dependence of recollision-enhanced multielectron effects in high-harmonic generation

Pragathi Darapaneni	Louisiana State University	Modifying the hybridization of transition metal d orbitals with weak external fields
Pu Du	Louisiana State University	A Coarse-Grained Model of N, N-dimethylacetamide: From Neat Liquid to Aqueous Solution
Qianyi Cheng	University of Memphis	Reaction Mechanisms of Benzylpenicillin Acylation and Deacylation with DD-peptidase
Reza Hemmati	Auburn University	An accurate benchmark description of chiral recognition in homo- and heterochiral dimers
Run Li	Florida State University	Development of Complex v2RDM Driven Relativistic CASSCF Methods
Sarah Johnson	University of Mississippi	Intermolecular interactions and vibrational perturbations in 1-ethyl-3-methylimidazolium thiocyanate / water mixtures
Holden Smith	Louisiana State University	Multi-Scale Modeling of Plasmon-Exciton Dynamics of Malachite Green Monolayers on Gold Nanoparticles
Thomas Ellington	University of Mississippi	Interrogating the Energetics and Vibrational Signatures of the H2-tagged N3-/H2O Complex
Thomas Summers	University Memphis	A Transition State “Trapped”? QM-cluster Models of Engineered Threonyl-tRNA Synthetase
Visal Kavinda Subasinghe Don	Louisiana State University	Graphene Oxide Liquid Interface - A Computational Study

Conference Venues

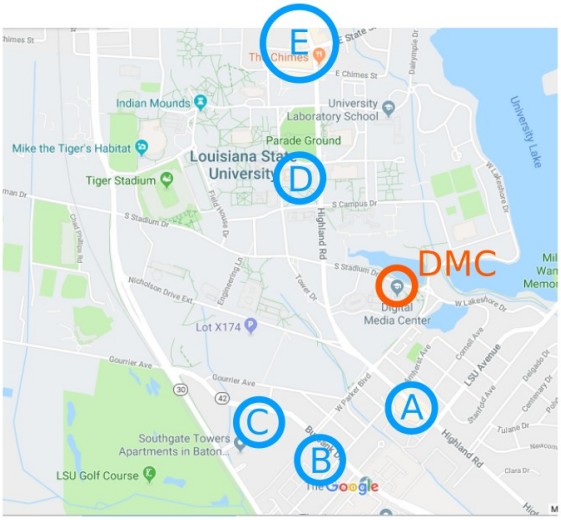
Andonie Museum (Banquet)

Digital Media Center (Registration and Presentations)



Parking

Lunch Suggestions (2 hours)



A (~ 8 min walk): Fat Cow Burgers, Drunken Fish (noodles and sushi)

B (~ 10 min walk): Izzo's Illegal Burrito, Mellow Mushroom (pizza)

C (~ 15 min walk): Breck's Bistro, LIT Pizza, Walk On's (bar)

D (~ 15 min walk): Student Union (various fast food)

E (drive recommended): The Chimes (bar), Chipotle, Kaminari (sushi and hibachi)