DE-SC0016316 Final Report

There were several prominent scientists from several countries and many excellent talks.
Several graduate students and postdocs were in attendance, some of whom were supported by the DOE 7557 funds.

List of attendees supported by the DOE 7557 funds:

The following received $1,000 each for travel support to the 7557 meeting
Tyanko Aleksev (graduate student – Zurich)
Colleen Bertoni (graduate Student – Ames)
Nuwan De Silva (postdoc – Ames)
Marilu Dick-Perez (postdoc – Ames)
Emilie Guidez (postdoc – Ames)
Kris Keipert (graduate student – Ames)
Tosaporn Sattasathuchana (graduate student – Zurich)
Ravithree Senanayake (graduate student – Kansas State)
Peng Xu (postdoc – Ames)
Aaron West (postdoc – Ames)

PROGRAM SCHEDULE for GAMESS7557 Meeting
January 15-18, 2016, Aqua Kauai Beach Resort, Lihue, Kauai

Sunday, January 15		Welcome Reception 5:00 – 7:00: Posters UP	
	All presentations 20 minutes		
Time	**Monday, January 16**	**Tuesday, January 17**	**Wednesday, January 18**
9:00-10:30	Chair: Brett Bode	Chair: Sarom Leang	Chair: Keiko Takano
	Klaus Ruedenberg Energy decomposition analysis of molecular wave functions	David Yarkony Accurate Nonadiabatic Dynamics	Pradipta Bandyopadhyay Water cluster and network in proteins
	Theresa Windus Computing Challenges: Today and Tomorrow	Sergey Varganov Nonadiabatic TST: Application to Intersystem Crossings in Active Sites of Metal-Sulfur Proteins	Jesse Lutz Recent Progress on SIMOMM/GAMESS
	Don Truhlar Recent Progress in DFT and Pair-DFT	Kazuo Takatsuka Chemistry of nonadiabatic electron flow	Emilie Guidez Theoretical bonding analysis of Si2H2 isomers
	Jay Siegel Assessing the importance of the Cation-Pi Effect	Cheol Ho Choi Exploring Nonadiabatic Dynamics with GAMESS	Hiroyuki Tamura Charge and Exciton Dynamics in Organic Photovoltaics
10:30-10:50	Coffee Break	Coffee Break	Coffee Break
10:50-12:15	Chair: Ivana Adamovic	Chair: Roger Amos	Chair: Bob Damrauer
	Benny Gerber VSCF in GAMESS and the Spectroscopic Determination of 3D Structures of Peptide Conformers	Joe O'Connor Metal-Accelerated Electrocyclization Reactions: Revelations from Theory and Experiment	Christine Aikens TDDFT Studies of Luminescence of Gold-Thiolate Nanoparticles
	Peter Gill MP2 energies, by Jove!	Tetsuya Takatsugu *Ab initio* MD study of branching reactions in the excited-state potential energy surface	Loîc Roch Implementation and Performance of Spin-Component-Scaled Double Hybrid DFT
	Piotr Piecuch Coupled-cluster interpretation of the photoelectron spectra of Ag_3 and Au_3	Sotiris Xantheas Aqueous solvation of multivalent metal ions: The role of excited states	Laura Zoppi First Principles Charge Transfer Excitations in Curved Aromatic Materials
	Angela Wilson Excited State Chemistry: From Electronic Structure to Electron Dynamics	Leo Radom Stabilities and Reactions of Free Radicals	Closing Ceremony
12:15-1:30	Lunch Break	Lunch Break	
1:30-3:00	Chair: Michael Schmidt	Chair: Larry Davis	
	Simon Webb Statistical Mechanics with Quantum Potentials: VM2-GAMESS	Lyudmila Slipchenko A journey with the Effective Fragment Potential method	
	Tosaporn Sattasathuchana Generalized Franck Condon Theory in GAMESS: Algorithm and Applications	Peng Xu Dispersion Interactions beyond r^6 term	
	Todd Martinez Nonadiabatic Dynamics From First Principles on GPU's	Dmitri Fedorov Analysis of interactions in complex systems	
	Ryan Olson GPU architectures, exascale and distributed tensors	Rika Kobayashi Fragmentation methods for diverse chemical properties	
3:00-3:30	Coffee Break	Coffee Break	
3:30-5:00	Chair: Kris Keipert	Chair: Paul Day	
	Alistair Rendell Low Power System-on-chip Processors for High Performance Computing: Achieving Energy Optimality	Kiet Nguyen Study of Linear and Nonlinear Optical Properties of Molecular Cadmium Chalcogenide Clusters	
	Jeongnim Kim From Future Architecture to Quantum Simulation Ecosystems	Joseph Ivanic Quantum Chemistry at the Frederick National Laboratory for Cancer Research	
	Tyanko Alekseev Arran: a highly available HPC system for reliable quantum chemistry calculations	Vanda Glezakou Marching towards task-specific materials using molecule simulations	
	Anna Krylov Two-photon absorption spectroscopy of molecular switches, insights from theory	Bun Chan Double hybrid DFTs and their applications to fullerene chemistry	
5:00-5:30	Break	Break	
	5:30–9:00: Banquet	5:30 – 7:00 Poster Session	