Computational Chemical Sciences Awards FY 2018

Lead PI	Institution	City, State	Proposal Title
Steele, Ryan	University of Utah	Salt Lake City, UT	Vibrational Signatures of Electronic Properties in Renewable-Energy Catalysis
Vlaisavljevich, Bess	University of South Dakota	Vermillion, SD	Controlling Molecular Structure and Spin with Multiconfigurational Quantum Chemistry
Car, Roberto	The Trustees of Princeton University	Princeton, NJ	Computational Chemical Science Center: Chemistry in Solution and at Interfaces
Caricato, Marco	University of Kansas Center for Research, Inc.	Lawrence, KS	Ab Initio Machine Learning Algorithms for Modeling Kinetics on Amorphous Catalysts
Lewis, James	West Virginia University Research Corporation	Morgantown, WV	Machine Learning for Excited-State Dynamics
Miller, Thomas	California Institute of Technology	Pasadena, CA	Ab initio Molecular Dynamics Beyond Density Functional Theory
Paesani, Francesco	The Regents of the University of California - UCSD	LA JOLLA, CA	Chemical Reactivity Through Adaptive Quantum Mechanics/Many-Body Representations: Theoretical Development, Software Implementation, and Applications
Peterson, Andrew	Brown University	Providence, RI	Bridging the time scale in exascale computing of chemical systems
Suryanarayana, Phanish	Georgia Tech Research Corporation	Atlanta, GA	SPARC-X: Quantum simulations at extreme scale - reactive dynamics from first principles
Gordon, Mark	Ames Laboratory	Ames, IA	Development of Exascale Software for Heterogeneous and Interfacial Catalysis