Department of Energy Announces $18.3 Million for Research to Develop Advanced Chemical Sciences Simulation and Modeling Capabilities

Annoucement Number: *DE-FOA-0002608* *List Posted:* *7/7/2022*

Principal Investigator	Title	Institution	City	State	9-digit zip code
Voth, Gregory	Multiscale Simulation Software for Energy Transduction in Biomolecular Systems: From Electrons to the Mesoscale	University of Chicago	Chicago	IL	60637-5418
Car, Roberto	Chemistry in Solution and at Interfaces (CSI)	Princeton University	Princeton	NJ	08540-2020
Gagliardi, Laura	Exascale Multireference Wave Function Theory Method for Polymer Upcycling Catalysis	University of Chicago	Chicago	IL	60637-5418
Gordon, Mark	Development of Exascale Software for Catalysis and Interfacial Phenomena	Ames Laboratory	Ames	IA	50011-1015
Suryanarayana, Phanish	SPARC-X: Quantum simulations at extreme scale – reactive dynamics from first principles	Georgia Tech Research Corporation	Atlanta	GA	30332-0420
Govind, Niranjan	Many-Body Methods, Spectroscopies, and Dynamics for Molecular Polaritonic Systems	Pacific Northwest National Laboratory	Richland	WA	99352-1793
Ping, Yuan	Spin-Selective Photocatalysis and Quantum Transport using Ab-Initio Density-Matrix Dynamics	University of California, Santa Cruz	Santa Cruz	CA	95064-1077
Hammes-Schiffer, Sharon	Multiscale Nuclear-Electronic Orbital Quantum Dynamics in Complex Environments	Yale University	New Haven	CT	06520-8327