Award Selection

The Office of Science of the Department of Energy is pleased to announce that 9 projects (listed below) have been selected to receive funding as part of competition for research in Computational Chemical Sciences sponsored by the Office of Basic Energy Sciences (a link to funding opportunity announcement can be located below). The research efforts will develop advanced software for the design of new chemicals and chemical processes for clean energy production and a range of other potential applications. A key aim of the current projects is to take full advantage of the nation's most advanced computers, including so-called "petascale" machines currently deployed at DOE national laboratories and the still faster "exascale" machines expected to be deployed beginning this year.

Projects announced at this time are selections for negotiation of financial award. The final details for each award are subject to grant and contract negotiations between DOE and the awardees.

Principal Investigator	Institution	City, State	Proposal Title
Jackson, Koblar	Central Michigan University	Mt. Pleasant, MI	FLO-SIC: Efficient Density Functional Theory Calculations
Krylov, Anna	University of Southern California	Los Angeles, CA	Novel Toolkit for Harnessing the Power of Exascale Computing for Catalyst Design
Siepmann, J. Ilja	University of Minnesota	Minneapolis, MN	Predictive Hierarchical Modeling of Chemical Separations and Transformations in Functional Nanoporous Materials
Sundararaman, Ravishankar	Rensselaer Polytechnic Institute	Troy, NY	Beyond-DFT Electrochemistry with Accelerated and Solvated Techniques (BEAST)
Valeev, Edward	Virginia Tech	Blacksburg, VA	Numerically-Exact Relativistic Many-Body Electronic Structure of Heavy Elements
van Schilfgaarde, Mark	National Renewable Energy Laboratory	Golden, CO	Hierarchical, Scalable Green's Function Modeling of Chemistry at Interfaces
Xantheas, Sotiris	Pacific Northwest National Laboratory	Richland, WA	Center for "Scalable Predictive methods for Excitations and Correlated phenomena" (SPEC)
Zádor, Judit	Sandia National Laboratories	Livermore, CA	Exascale Catalytic Chemistry (ECC) Project 2021
Zimmerman, Paul	University of Michigan	Ann Arbor, MI	From Wave Functions to Exchange Correlation for Large-Scale Electronic Structure

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