Award Selection

The Office of Science of the Department of Energy is pleased to announce that 5 projects (listed below) have been selected to receive funding as part of competition for research in the Scientific Discovery through Advanced Computing (SciDAC) program sponsored by the Offices of Advanced Scientific Computing Research (ASCR) and Basic Energy Sciences (BES) (a link to funding opportunity announcement can be located below). The research efforts will support integrated teams of researchers to address energy-relevant topics of quantum phenomena in many-particle systems driven far from equilibrium, and predictive control of reaction pathways for chemical mechanisms in complex non-equilibrium and field-driven environments. SciDAC brings together experts in key areas of energy research, computational chemical and materials sciences with experts in applied mathematics, and computer science to take maximum advantage of high-performance computing resources. The teams will partner with either or both of the SciDAC Institutes FASTMath and RAPIDS2 led by Lawrence Berkeley and Argonne National Laboratories.

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

Principal Investigator	**Institution**	**City, State**	**Proposal Title**
Chan, Garnet	California Institute of Technology	Pasadena, CA	Traversing the “death valley” separating short and long times in non-equilibrium quantum dynamical simulations of real materials
De Prince, Albert	Florida State University	Tallahassee, FL	Relativistic Quantum Dynamics in the Non-Equilibrium Regime
Head-Gordon, Martin	Lawrence Berkeley National Laboratory	Berkeley, CA	Large-scale algorithms and software for modeling chemical reactivity in complex systems
Vlcek, Vojtech	University of California, Santa Barbara	Santa Barbara, CA	Real-time dynamics of driven correlated electrons in quantum materials
Wong, Bryan	University of California, Riverside	Riverside, CA	DECODE: Data-driven Exascale Control of Optically Driven Excitations in Chemical and Material Systems

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