Energy Department to Invest $32 Million in Computer Design of Materials

Researchers to Take Advantage of DOE's Advanced Supercomputer Capabilities

WASHINGTON—The U.S. Department of Energy announced today that it will invest $32 million over the next four years to accelerate the design of new materials through use of supercomputers.

Seven projects will be supported, three led by teams at DOE National Laboratories and four by Universities. The teams are led by Argonne National Laboratory (ANL), Brookhaven National Laboratory (BNL) and Lawrence Livermore National Laboratory (LLNL) as well as the University of Illinois, the Pennsylvania State University, the University of Texas and the University of Southern California.

Details of the awards selected for negotiation are shown below:

PI	Institution	City, State	Proposal Title
Ceperley, David	University of Illinois	Champaign, IL	From accurate correlated quantum simulations to mesoscopic scales
Chen, Long-Qing	Pennsylvania State University	University Park, PA	Computational mesoscale science and open software for quantum materials
Galli, Giulia	Argonne National Laboratory	Lemont, IL	Midwest integrated center for computational materials (MICCoM)
Giustino, Feliciano	University of Texas at Austin	Austin, TX	Toward exascale computing of electron-phonon couplings for finite-temperature materials design
Kotliar, Gabriel	Brookhaven National Laboratory	Upton, NY	Comscope: Center for computational design of functional strongly correlated materials and theoretical spectroscopy
Ogitsu, Tadashi	Lawrence Livermore National Laboratory	Livermore, CA	Center for non-perturbative studies of functional materials under non-equilibrium conditions (NPNEQ)
Vashishta, Priya	University of Southern California	Los Angeles, CA	Materials genome innovation for computational software (MAGICS) center