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.

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