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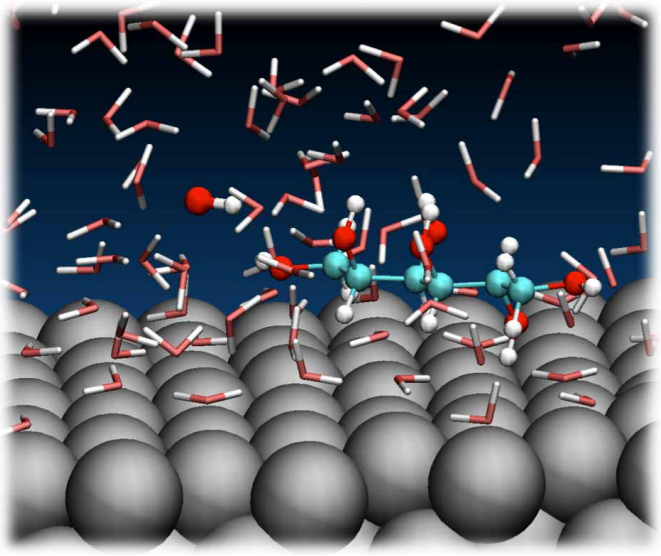
SDSC Announces International Chemistry Collaboration

Simulations to Aid Fuels and Chemicals Research



Example of bifunctional catalysis. A platinum surface and hydroxide ion in aqueous solution catalyze the transformation of sorbitol into more valuable chemical compounds. Sorbitol is an example of a sugar molecule that can be extracted from renewable biomass. Platinum atoms are depicted as gray balls, carbon atoms are cyan, oxygen atoms red, and hydrogen atoms white. The triangles represent water molecules. Image: Andreas Goetz/SDSC.

The San Diego Supercomputer Center (SDSC) at the University of California, San Diego is a partner in a new international collaboration to develop computational models and software for simulations of bifunctional catalysis, which is of high relevance for biomass conversion to liquid fuels and raw materials used in the chemical industry.

The research is co-funded by a three-year award from the National Science Foundation's Divisions of Chemistry (CHE) and Advanced Cyberinfrastructure (ACI), and the French National Research Agency (ANR), with the combined award valued at almost $815,000 (EUR 706,000.) Three institutions are involved in the collaboration: SDSC and the University of Delaware in the U.S., and the École Normale Supérieure de Lyon in France, bringing together research teams with complementary expertise.

"Detailed computer simulations can play a key role in understanding how these catalysts function at a molecular level and guide the development of improved catalysts for industrially viable processes in biorefineries," said principal investigator Andreas Goetz, an SDSC researcher with expertise in molecular dynamics simulations and multiscale quantum mechanics/molecular mechanics (QM/MM) algorithms. "These simulations are computationally

very demanding, and SDSC's new *Comet* supercomputer, with its advanced Intel Haswell CPUs and NVIDIA Kepler GPUs, will be an extremely valuable resource for code development and numerical simulations of this project."

While bifunctional catalysts are important for the conversion of oxygen-rich compounds sourced from biomass into liquid fuels and valuable chemical feedstocks, several computational models need to be improved and combined in order to address the complexity inherent to the catalytic processes of bifunctional catalysts in solution.

"This international collaboration is a unique opportunity to build on complementary expertise available in different labs, ranging from heterogeneous catalysis to multiscale simulation models and software development," added Goetz. "This work is important to support a sustainable future that does not rely on dwindling petroleum resources, while reducing carbon dioxide emissions and minimizing global warming. Also, this research and its methods could be applied to multiple fields of study ranging from chemistry and chemical engineering to the biosciences."

The researchers plan to integrate new multiscale methods into freely available open source software libraries and distribute them with AMBER, a widely used molecular simulation package. Other members of the research team include Dionisios G. Vlachos from the University of Delaware, and Philippe Sautet, Paul Fleurat-Lessard, and Carine Michel of the École Normale Supérieure de Lyon in France.

The NSF portion of the grant for the research with the title 'International Collaboration in Chemistry: CDS E: Multiscale Simulations of Bifunctional Catalysis' is funded under NSF award numbers 1416571/1415828 and runs until the end of 2017.

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