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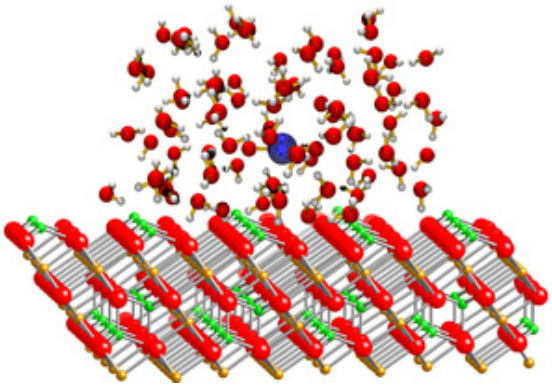
EMSL In Brief
Environmental Molecular Sciences Laboratory

Supercomputing Resources Brave the Heavy Elements

A research team composed of scientists from the Environmental Molecular Sciences Laboratory (EMSL), Idaho National Laboratory, and Wichita State University is uniting theory, computation, and experiment to discover exactly how heavy elements, such as uranium and technetium, interact in their environment.

As part of that effort, the team combined sensitive experimental measurements with first principle electronic structure calculations to measure—and really understand—the structural and bonding parameters of uranyl, the most common oxidation state of uranium in systems containing water. Their insights were achieved using EMSL's high-performance computational resources.



Researchers are discovering how actinides such as uranium in solution interact with their environment.

The large number and behavior of electrons in heavy elements makes most of them extremely difficult to study. According to de Jong, lead of EMSL's High-Performance Software Development group and a member of the team, advancements in computing power and theory are enabling computational actinide chemistry to contribute significantly to the understanding and interpretation of experimental chemistry data, as well as to predicting the chemical and physical properties of heavy transition metal, lanthanide, and actinide complexes.

"Now we can make sure we get the right answer for the right reason," de Jong said, adding that results obtained from the calculations are an invaluable supplement to current, very expensive, and often hazardous experimental studies.

Discoveries made using the new capabilities available to the growing field of computational actinide chemistry could have wide impact, from radioactive waste and cleanup challenges to the design and operation of future nuclear facilities.

Bert de Jong presented the team's findings at the 234th American Chemical Society National Meeting in Boston this August.

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