Scientists Show Strontium's Swimming Skills

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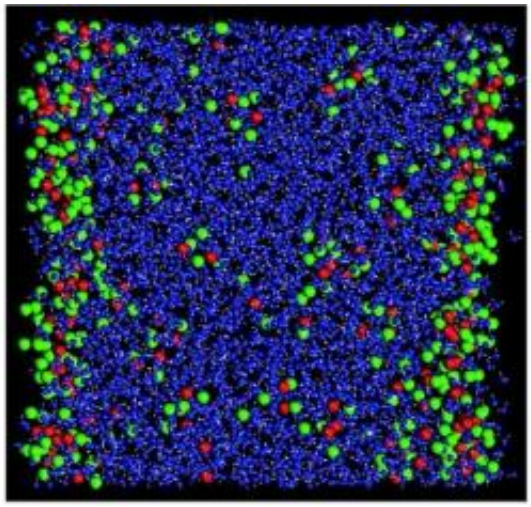

Snapshot from the simulations with the polarizable potential. Water molecules are in blue. The Cl- ions are in green and the corresponding Sr2+ ions are in red.

(PhysOrg.com) -- Recently, a trio from Pacific Northwest National Laboratory and Louisiana Tech University showed that strontium ions congregate on water's surface. Their computer simulation and careful calculations finally demonstrated why experiments and conventional wisdom clashed about the behavior of this type of ion, a divalent cation or one with two electrons missing.

Understanding ions behavior where air and water meet is vital to predicting and eventually controlling chemical reactions, whether those reactions form clouds or produce fuels. However, this understanding has to be accurate. When measurements from experiments do not agree with

the current understanding, well, that's where theoretical chemists with good modeling skills come in.

For years, the conventional wisdom was that cations fled from the surface of water or the aqueous interface. But, experiments with x-ray relectivity contradicted this view. So, PNNL postdoctoral fellow Dr. Xiuquan Sun, Dr. Liem Dang, also of PNNL, and Dr. Collin Wick of Louisiana Tech University decided to see if they could figure out what was happening.

They chose to study strontium ions, which come from strontium chloride ($SrCl_2$) dissolved in water. Strontium is a divalent cation, with two positive charges. It behaves differently than sodium or other ions with only a single positive charge.

For the simulation, they used a molecular dynamics approach. This approach is a computer simulation that allows the tiny, fast-moving ions and water molecules to interact based on the laws of physics. The investigators record these interactions, which happen within a split second. Then, they can calculate the density of the electrons at the surface and the structures that are forming there and see how close the calculations come to what was measured during the x-ray reflectivity experiments.

One parameter the team checked was if the model's representation of the shape of the electron cloud around the ion mattered. Electrons are the fast-moving negative particles that zoom around an ion.

In one series of simulations, the researchers considered that the electron cloud might not be a perfect sphere around the ion and solvents. Other ions and molecules might distort the cloud. This was called the polarizable potential model. In another series of simulations, they did not include the electron cloud around the ion and solvent. This was the

nonpolarizable potential model.

The team found that the polarizable approach provided better results, more closely matching the data from the x-ray reflectivity experiments. So, using the polarizable model, they calculated where the electrons congregated and the resulting structures created on the surface of the water. They found that the strontium ions strongly prefer to congregate on the surface, just as the experiments showed.

However, the results from the approach were far from perfect. At low concentrations of strontium ions, the researchers find good agreement with the experiments, but at higher concentrations, the molecular models overestimate the surface concentration by around a factor of 2. So, the team is refining the models to get better agreement at higher concentrations.

More information: Sun X, CD Wick, and LX Dang. 2009. "Computational Studies of Aqueous Interfaces of SrCl2 Salt Solutions." *Journal of Physical Chemistry B*. DOI: 10.1021/jp9079525

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