Computational Chemistry's Insatiable Hunger For Computer Resources

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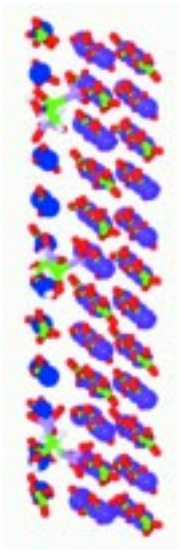

Ball and stick graphical representation showing how HEDP ions fit into steps on a calcite surface

Assume that there exists a scientist who would like to simulate the movements of one mole (18 centi-litres) of water at room temperature and pressure. Treating the water molecules as rigid bodies this gives

6 * 6.023*10^23 degrees of freedom in the simulation. To count from one to

6 * 6.023*10^23 using 512 processors on turing would take at least 186 480 years, this is assuming that every instruction issued is used to increase the count by one.

Our droplet researcher was presumably planning to use classical mechanics to describe the motions of the water molecules.

According to classical mechanics chemical reactions cannot take place if matter is quantized. Many 19th century physicists were therefor critical of Dalton's atomic theory and preferred things like mathematically incomprehensible continuum models suffering from vortex knots. Today there is quantum mechanics, also mathematically incomprehensible, which does allow for atoms to undergo chemical reactions and form complicated molecules.

With chemical reactions theoretically allowed it is reasonable to hope that they can be understood by bone-headed calculation. High accuracy quantum mechanical calculations do in practice struggle with the reaction:

H_2 + O ==> H_2O

and an entire fauna of approximative methods have evolved. A popular choice is to revert to classical mechanics when all chemical bonds are expected to remain intact. An example of what can be done with calculations employing classical mechanics is shown in the picture.

This ball and stick graphical representation shows how HEDP ions fit into steps on a calcite (CaCO3) surface. Using the good, old trial and horror procedure it has been empirically established that HEDP ions stop calcite crystal from growing. It is also known that the major growth mode of calcite is to add material at steps on the surface. From this it can be figured that HEDP ions ends at the surface doing something, but where did they go and what do they do?

The HEDP ion can enter into a calcite surface by replacing two carbonate ions without breaking or forming any chemical bonds and this process can thus be descibed with reasonable accuracy using classical mechanics. Using classical mechanics, it can be well described which the surface sites that HEDP ions prefers to bind to are. From these calculations it was learned that HEDP ions prefers to be at step sites, as shown in the picture, over the flat surface. Once anchored to the step, the HEDP ion prevents calcium and carbonate ions from binding to the step, thereby poisoning crystal growth.

These calculations, done by researchers at the Royal Institution in London and Curtin University in Perth, Australia, used up several CPU months on Origin 2000 and CRAY-T3E systems. It would of course be very interesting to include water-surface interactions into these simulations. To be able to predict the growth inhibiting properties of various ions, rather than just explain how they work, it would also be necessary to include protonation and deprotonation reactions of anions in aquatic solution. If adequate computational resources had been available; these calculations would, of course, have been undertaken.