NSC News
National Supercomputer Centre at Linköpings universitet
2006:2

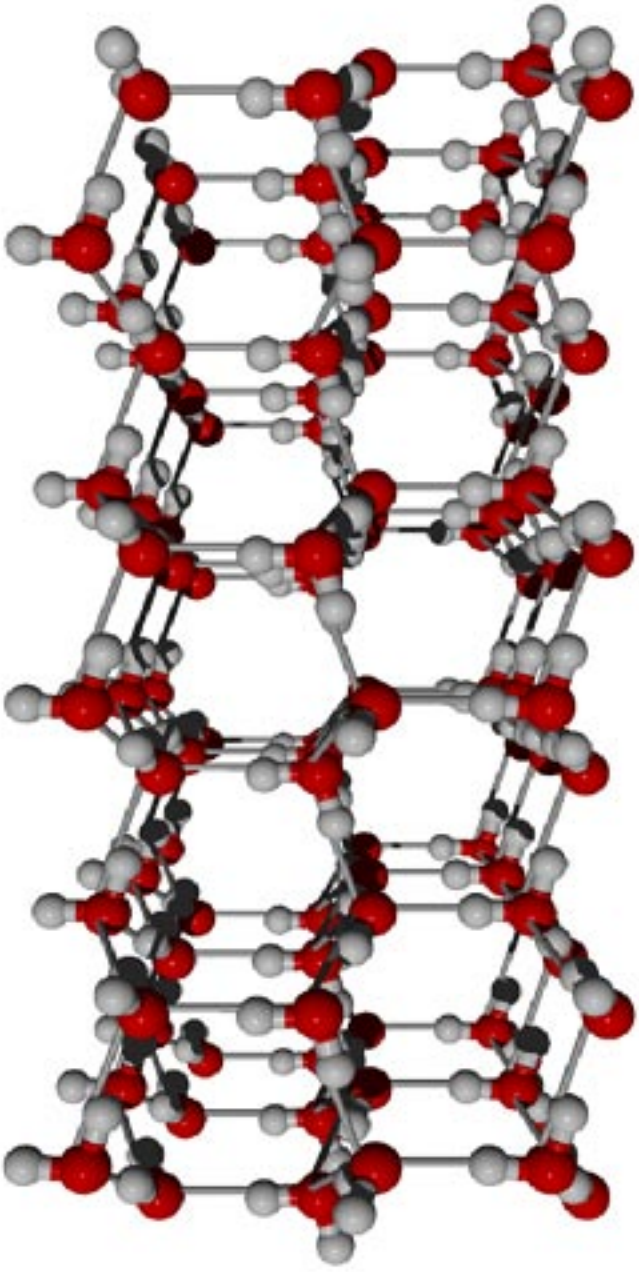

Figure 1a) The structure of ice XI.

Plain as water

Sometimes ice is not just ice. And nanoscale particles can behave very differently from the same material in bulk form.

Lars Ojamäe has been using the Sgi3k, Monolith and Mozart systems at NSC to study the properties of water ice in different phases. He also explores how coating nanocrystals with organic molecules can improve MRI examinations and help us build better solar sells.

Read further on page 3

The Stakkato intrusions

Remember the big wave of intrusions that hit hundreds of universities, HPC centres and other sites during 2004 and early 2005?

During the Cluster Security workshop at CCGrid06 in Singapore, NSC systems expert Leif Nixon spoke about what really happened and how the perpetrator was finally tracked down.

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Mozart highly sought after

In the latest SNAC application round, NSC's new SGI Altix system, Mozart, received applications for more than six times the available amount of computation time.

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Great expectations for the future

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It is probably a very nice feeling to go on vacation with an "empty desk", but we all know that it usually does not happen. Instead, we have to spend the first working days after summer vacation trying to remember the details of the work tasks that were so familiar to us before summer. But after all, that is the whole idea with vacation, to relax and forget about work. Another good side of it is that leaving the work tasks for a while will probably result in new ways to look at them, and eventually to better solutions.

Which are the ongoing work tasks at NSC? As usual, we put operations and support at the top of our priority list and these tasks will go on as usual, but of course with some reduction in manning during July. Concerning development projects, our main focus is to find the successor to Monolith. Even though in the last round of SNAC applications Monolith was as popular as ever, we know that the system is approaching the end of its lifetime and it will be taken out of service as a SNAC resource one year from now. We have sent a proposal to SNIC for a new resource and we are confident that the HPC solution that we are describing in this proposal can become the most useful ever for the Swedish HPC community. If granted, the new resource will be available to SNAC users starting from July 1, 2007. LiU has just approved the setup of a new computer building, which will be nearly 4 times as large as the present one. This is one of the most important steps taken in order to ensure that NSC remains the leading Swedish HPC centre; during the next couple of years we expect to have the necessary infrastructure to host new HPC systems for SNIC, SMHI, and the Nordic WLCG Tier 1.

Last month I visited the DEISA (Distributed European Infrastructure for Supercomputing Applications) symposium in Bologna. It was a very interesting meeting, in particular the presentations of the application projects were fascinating and stimulated a lot of thinking concerning the Swedish HPC community. There are 27 DEISA projects (http://www.deisa.org/applications/projects2005-2006/). Unfortunately, the Swedish participation is very limited. I think that we have very strong national candidates that could compete at the European level for the kind of resources that are offered within DEISA. I am not writing this to encourage our users to leave NSC for other resources. On the contrary, if Sweden can show that we have top level researchers this will increase the national level of funding and eventually we (NSC) can take part in DEISA as a provider of resources.

With these exciting possibilities for the future in mind, I would like to wish all my colleagues at NSC and LiU and all our users and partners a very nice and relaxing summer!

Cluster-Sec'06 at CCGrid06

The second Cluster Security workshop was held in May in conjunction with the CCGrid06 conference in Singapore.

One of the recurring themes of the workshop, indeed of the entire conference, was how virtualization can be used as a tool for security-related sandboxing, for OS provisioning on demand and for application deployment. Virtualization techniques will no doubt continue to attract interest in the HPC world, as well as in corporate enterprise data centers.

The keynote talk of Cluster-Sec'06 was given by NSC systems expert Leif Nixon, who talked about the Stakkato intrusions. In June 2004 NSC systems were out of service for several weeks after two intrusion incidents. These turned out to be just a small part of a huge wave of attacks, where stolen ssh passwords were used to gain illegal entry to hundreds of sites, including CERN, MIT, Stanford, US military installations and most Swedish universities. Leif told the story about what really happened and how the intruder was finally tracked down and caught.

The slides from the talk can be found at http://www.nsc.liu.se/~nixon/stakkato.pdf

LCSC
7th annual workshop on
Linux Clusters for Supercomputing

Linköping October 17–18 2006
http://www.nsc.liu.se/lcsc/

Water and functionalized nanocryst

What the structures of nanoparticles look like, how they interact with organic molecules, and their potential applications in medicine, chemical sensors and solar cells, along with how H-bond topologies can be related to thermodynamic stabilities of ice crystals and water clusters. These are examples of issues within the physical-chemistry field that we study using computational-chemistry methods and the computational resources of NSC.

Ice and water clusters

In a true crystal the atoms are ordered in a regular and repeating pattern. In ordinary ice, ice Ih, the oxygen atoms are ordered, but the hydrogens of each water molecule may point more or less randomly in different directions to the neighbouring molecules. The crystal is said to be proton-disordered. Linus Pauling derived an expression for the maximum proton disorder already in the 1930's, but the factual degree of disorder remained beyond the theoreticians' reach. It has been debated whether ice Ih ever forms a perfect crystal. According to some experiments the proton-ordered crystal, termed ice XI, will be formed at a temperature below –200°C, whereas others have indicated a phase transition at a much higher temperature. Even the experimentally suggested structure of ice XI (whose cell's net dipole moment categorizes it as ferroelectric, Fig. 1a on page 1) has been criticized and branded as "underidentified ferroelectric ice" or "UFI".

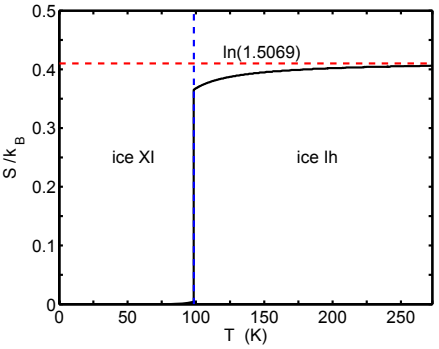

Figure 1b) The configurational entropy versus temperature for ice obtained from MC simulations.

Theoretical calculations for proton-disordered ice is complicated by the fact that even for moderately-sized unit cells the number of possible H-bond arrangements soon becomes gigantic, and at the same time the energy differences between different orientations are tiny, so highly accurate (i.e. quantum-chemical) and time-consuming computations are needed. To model the order-disorder phase transition we therefore use a combination of theoretical methods. From a graph-theory point of view, each H-bond arrangement can be seen as a directional graph, and at first all such possible H-bond topologies of small given unit cells were generated. For these it was possible to perform quantum-chemical periodic DFT calculations using the Sgi3k and Monolith systems (we noted a nice agreement between relative lattice energies obtained from different DFT codes such as CPMD, CASTEP, DMol3 and CRYSTAL once the program settings been trimmed to highest precision). By analysing the different H-bond topologies to identify structural characteristics, we derived parametric relations between topology and lattice energy. Finally, by utilizing these in Monte Carlo simulations the thermodynamic properties are computed.

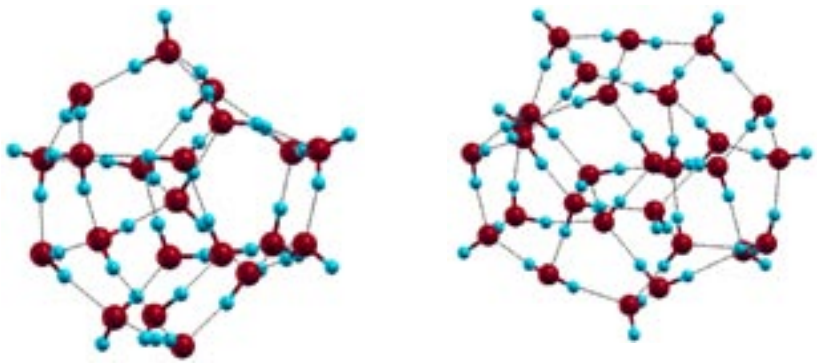

Figure 2. Water clusters consisting of a) 21 and b) 28 water molecules.

Mozart, popular from the start

The new shared memory system Mozart at NSC has turned out to be very attractive for HPC users in Sweden right from the start. In total 132 400 hours/month was applied for from the Swedish National Allocations Committee, SNAC, which is more than six times the 21 000 hours/month available in the current application round. The SNAC committee thus has to carefully judge, in addition to the scientific merit, the need for the unique large shared memory of Mozart when evaluating the applications.

It is also pleasant to see that Monolith continues to be a valuable resource to the Swedish HPC-community despite its age. The total time applied for, 319 267 hours/month, is more than two and a half times the time available for allocation.

On Swegrid, which NSC operates the Bluesmoke node of, the total time applied for was moderately higher, about 25%, than the available time.

The calculations correctly predict the ferroelectric ice XI structure to be the most stable of practically all H-bond topologies. Most important, from the variation of entropy with temperature (Fig. 1b), an order-disorder phase transition is demonstrated to occur and the transition temperature established to be close to −200°C. The entropy is found to be slightly lower than the Pauling estimate even near the melting temperature, which implies ordinary ice to be more ordered than expected.

It follows that ice on Earth should be proton-disordered. But on other celestial bodies, like Jupiter's moon Europa and in comets, phase transitions to the ordered form will take place.

In the atmosphere water $(H_2O)_n$ (Fig. 2) and protonated water $H^+(H_2O)_n$ clusters participate in environmentally important chemical reactions, such as the ozone depletion mechanism.

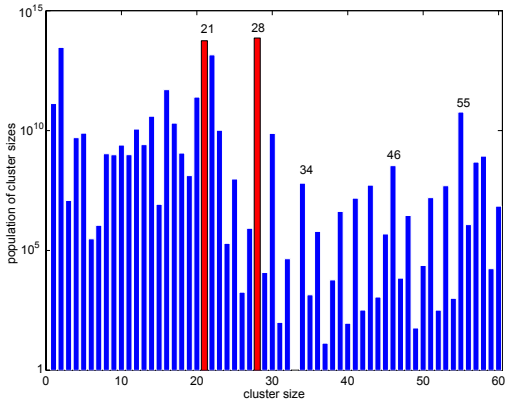

Figure 3. Distribution of water clusters of various sizes at 1 atm and 200K (the peaks marked by red constitute experimental magic numbers).

Quantum-chemical ab initio calculations and MC/MD simulations (sporting our polarizable and dissociative water potential model) have been used to describe the structure and dynamics of such clusters.

A central idea of this study is to find out how the stabilities of the clusters are related to their H-bond topologies. From GAUSSIAN computations using MP2/MP4 or B3LYP and large basis sets, reliable cluster structures and formation energies were obtained (for the large clusters the use of the shared-memory and multi-processor Mozart platform is indispensable), and it is found that the topology indeed significantly governs the stabilities. By a proper inclusion of the H-bond statistics, dynamical effects and thermodynamic equilibria, it is possible to reproduce qualitatively the "magic numbers" observed in mass spectra of ionized clusters (Fig. 3). This in turn is a strong indication that the computed structures are correct.

"It follows that ice on Earth should be proton-disordered."

Nanocrystals functionalized by organic adsorbates

The term nanoparticle refers to particles of dimensions 1–100 nm, and matter in this form may possess mechanical, optical and electronic properties that differ significantly from when present in its molecular or bulk forms. Metal-oxide nanocrystalline particles are attracting interest due to their usage and potential capabilities as for example dye pigments, heterogeneous catalysts, chemical sensors and biomarkers, light-emitting devices and photodetectors, and solar cell components.

The properties of the nanocrystals can be further modified by capping the surface with an organic molecular layer, which interacts with surface states of the metal oxide. The adsorbed molecular layer may in turn contain functional groups that carry out a desired action, for example attachment to a specific target or absorption of light of a certain wavelength.

A possible medical application is to use magnetic nanocrystals as contrast agents in magnetic resonance imaging (MRI). Complexes containing gadolinium are used today in MRI examinations of patients, where the contrast ability stems from the paramagnetic properties of Gd. As an alternative to Gd complexes the nanocrystalline oxide,

Nordic WLCG Tier 1 activities

NSC, together with PDC in Stockholm, HPC2N in Umeå and NBI in Copenhagen, is participating in CERN's Service Challenge 4, which is a ramp-up to the production stage of WLCG, the Worldwide LHC Computation Grid.

WLCG will be used to store and analyze the extremely large streams of data that will be generated by CERN's new LHC accelerator when it goes online.

The goal of Service Challenge 4 is to validate the ability to stream 1 GB/s from CERN to eleven designated Tier 1 sites around the world, with NSC, PDC, HPC2N and NBI appearing as a distributed Nordic Tier 1 site under the umbrella of NDGF, the Nordic Data Grid Facility, which represents the collected national grid projects in the Nordic countries.

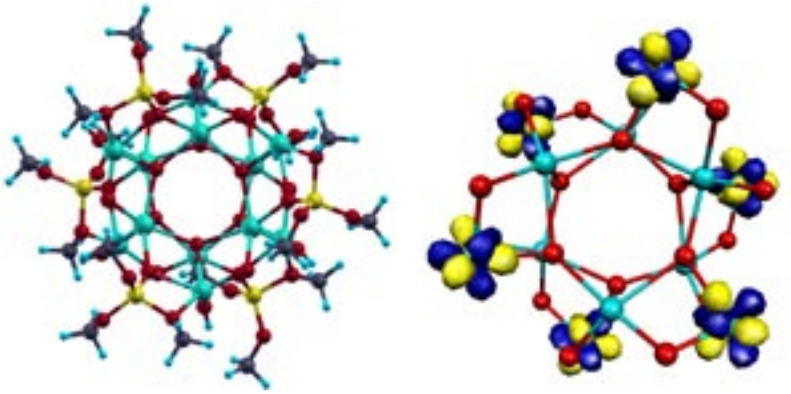

Figure 4. a) A Gd_2O_3 nanoparticle capped by a layer of tetramethoxysilane. b) Gd f-orbitals in the nanoparticle.

Gd_2O_3, has been suggested. For use in vivo the nanocrystals can feasibly be bio-functionalised by coating by a biocompatible molecular layer.

We have studied the chemisorption of various organic molecules, e.g. citric acid, diethylene glycol and tetramethoxy silane, on Gd_2O_3 nanocrystals (Fig. 4). Detailed information on the molecule-nanocrystal interactions such as adsorption energies and coordination geometries, not readily obtained experimentally, are extracted from quantum-chemical calculations. The agreement between computed and experimental IR or UV/Visible spectra helps to validate the proposed structure models. It turns out that the electronic structure of the surface region, predominant in these small clusters, greatly affects their properties. At least the particles of sizes close to 1 nm appear to be in a high-spin state. Each particle thus behaves as a ferromagnet. A possibility is that in a diluted liquid suspension they are randomly oriented, but an imposed magnetic field would cause an alignment of the nanosized magnets to create a superparamagnetic effect, which boosts the contrast capability.

In collaboration with Sten Lunell in Uppsala and Petter Persson in Lund we are studying nanostructured dye-sensitized solar cells. Ordinary metal oxides have too wide band gaps to absorb visible light efficiently, but in dye-sensitized solar cells the longer wavelengths can be harvested by coating the nanocrystalline metal oxide (e.g. TiO_2) by a molecular dye (usually a Ru^{2+}-bipyridine complex). The excitation energy is lower in the dye, and the molecular excitation is followed by an electron injection from the dye to the metal oxide's conduction band.

We study the dye adsorption process and electron-injection mechanism for model dyes adsorbed on TiO_2 and ZnO surfaces (Fig. 5). We use periodic B3LYP computations, where we benefit from the accurate band gaps obtained from this method. In the solar cell the dye binds to the surface through anchor groups. It is found that phosphonic acid provides a significantly stronger bond than the commonly used carboxylic acid. Visualization of the LUMO orbitals and inspection of DOS spectra reveal strong electronic coupling between adsorbate and metal-oxide substrate. Computed injection times are in the 10–40 fs regime, where the carboxylic anchor enables twice as fast electron transfer compared to phosphonic acid. Such information may ultimately aid the construction of novel solar cells.

We are indebted to PhD students Annika Lenz, Henrik Pedersen, and Mattias Nilsing (UU) for providing results and pictures.

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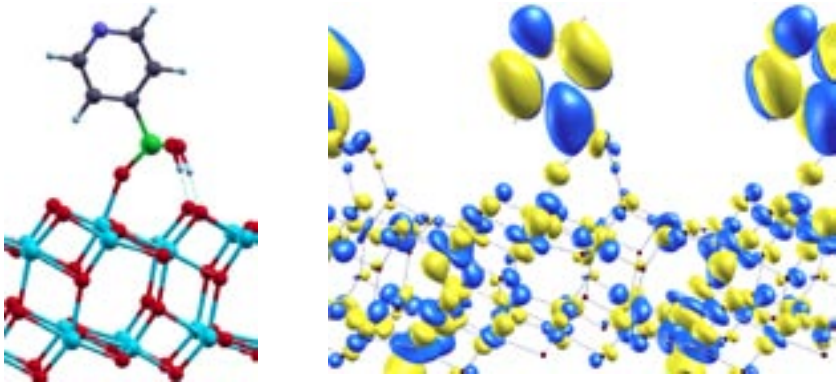

Figure 5. The optimized structure and the lowest unoccupied orbital associated with the molecule for pyridine-4-phosphonic acid adsorbed on an anatase surface from periodic B3LYP calculations.

Lars Ojamäe is associate professor and senior lecturer in physical chemistry, especially computational chemistry. He got his PhD in 1993 at the department of inorganic chemistry, Uppsala University, and then did a postdoc with Isaiah Shavitt at the Ohio State University, USA, followed by a Marie Curie-fellowship visit with Cesare Pisani in the University of Turin, Italy. During 1996–2001 he was assistant professor at the physical chemistry department, Stockholm University. In 2001 he joined the faculty at Linköping University.

UPCOMING EVENTS

International Workshop on High-Level Languages, Compilers, and Tools for Parallel Programming

June 13, 2006, Linköping, Sweden. http://www.ida.liu.se/~chrke/workshop-060613/

PARA'06; Workshop on state-of-the-art in Scientific and Parallel Computing

June 18–21, 2006, Umeå, Sweden http://www.hpc2n.umu.se/para06/

HPDC-15; The 15th IEEE International Symposium on High Performance Distributed Computing

June 19-23, 2006, Paris, France. http://hpdc.lri.fr

CLADE 2006; Challenges of Large Applications in Distributed Environments

Held in conjunction with HPDC-15. June 19–20, 2006, Paris, France. http://www-unix.mcs.anl.gov/~bair/CLADE2006/

ISC 2006; International Supercomputer Conference

Juny 27–30, 2006, Dresden, Germany. http://www.supercomp.de/

ICPADS 2006; 12th International Conference on Parallel and Distributed Systems

July 12–15, 2006, Minneapolis, Minnesota, USA. http://www.icpads.umn.edu/

WoCo9: IFIP Working Conference on Grid-based Problem Solving Environments: Implications for the Development and Deployment of Numerical Software

July 17–21, Prescott, Arizona, USA. http://www.woco9.org/

ICPP 2006; The 2006 International Conference on Parallel Processing

August 14–18, 2006, Columbus, Ohio, USA. http://www.cse.ohio-state.edu/~icpp2006

Euro-Par 2006; European Conference on Parallel Computing

August 29–September 1, Dresden, Germany. http://www.zhr.tu-dresden.de/Euro-Par2006/

PARELEC; 2006 IEEE International Conference on Parallel Computing in Electrical Engineering

13–17 September, Bialystok, Poland http://we.pb.bialystok.pl/~parelec2006/

EuroPVMPI'06; European PVM/MPI Users' Group Meeting

September 17–20, 2006, Bonn, Germany. http://www.pvmmpi06.org/

Cluster 2006; IEEE International Conference on Cluster Computing

September 25–27, 2006, Barcelona, Spain. http://www.cluster2006.org/

GRID 2006: The 7th IEEE/ACM International Conference on Grid Computing

September 28–29, 2006, Barcelona, Spain. http://www.grid2006.org/

NPC 2006 IFIP International conference on on Network an Parallel Computing

October 2–4, Tokyo, Japan. http://www.npcconf.org/

LCSC; 7th Annual Workshop on Linux Clusters for Supercomputing

October 17–18, 2006, Linköping, Sweden. http://www.nsc.liu.se/lcsc/

SC 06; International Conference for High Performance Computing, Networking, Storage and Analysis

November 11–17, 2006, Tampa, USA. http://sc06.supercomputing.org/

HiPC 2006, 13th IEEE International Conference on High Performance Computing

December 18 -21, 2006, Bangalore, India. http://www.hipc.org/

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