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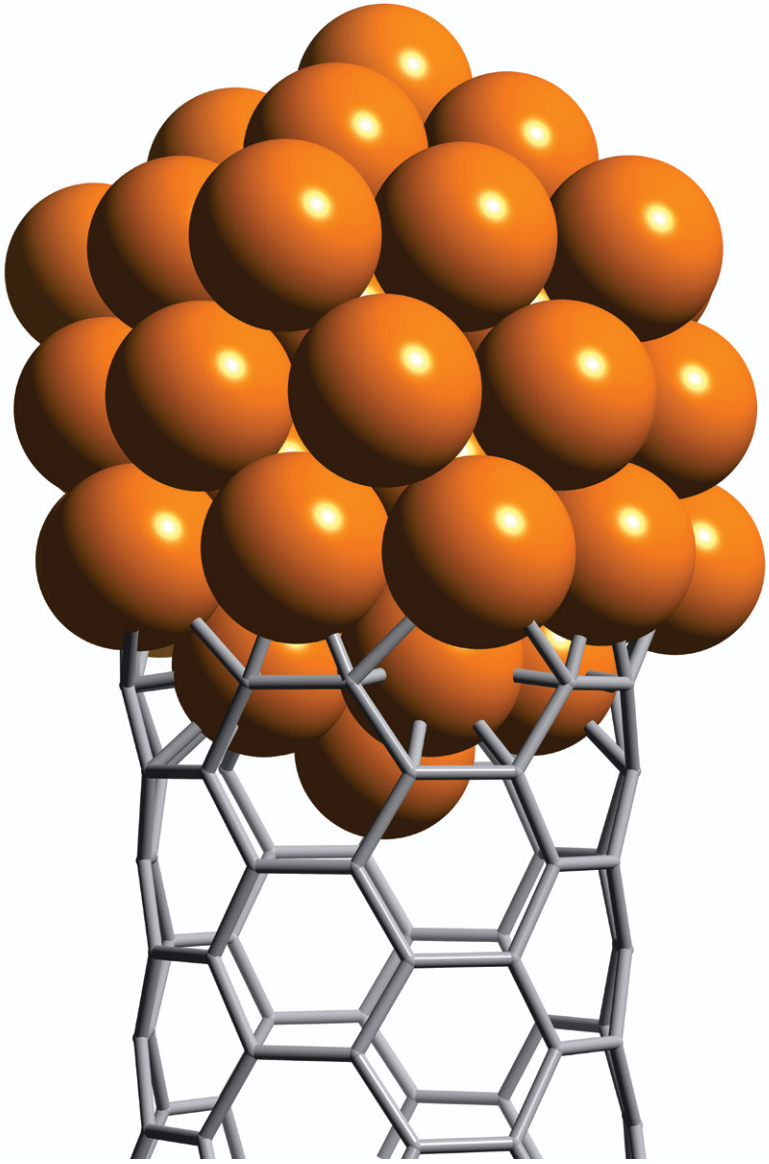
National Supercomputer Centre at Linköpings universitet

20 YEARS IN HPC 1989–2009



Materials Science

Computational Materials Science from *ab initio*

Rajeev Ahuja use state-of-the-art theoretical methods to tackle complex material science systems at a very hight level of detail.

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Press Stop

"One of the most important problems in materials science solved" says Professor Peter Oppeneer of Uppsala University.

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20 YEARS IN HPC 1989–2009

It's time to celebrate the 20th year anniversary of NSC. In practice the centre became operational when the four-processor Cray X-MP/48 vector supercomputer was installed in April 1989 and made available to academic and industrial users. These events were preceded by more than one year of hectic preparations – during this period the centre emerged step by step. Important activities were how to secure funding, organise the centre, fix networking, security etc. And most important, how Linköping University would win the open national competition for a new national supercomputer centre. This race was fierce, sometimes rude and much enjoyed by mass media. Previous to NSC there was a CRAY-1 owned by Saab Scania AB. Through NFR this computer was to a limited extent available also to academic users. This joint arrangement obviously contributed to the credibility of the Linköping proposal to run a fully academic centre.

Depending on your perspective twenty years may seem very long or short. If you are a young student today 1989 is "prehistoric" and easy access to inexpensive high-performance computing and associated services is taken for granted. If you have been in the game for a longer time, perhaps to the extent that you are now "historic", you may be more humble as you have witnessed the enormous development over these twenty years, a development that was hardly foreseen. One should recall that in the eighties the Swedish university network SUNET transmitted at 64 kbit/s or less. Terminals were available, but workstations and interactive web-services were still in its infancy. Security rules for accessing supercomputers were rather forbidding, basically because of the cold war. This affected the choice of the operational system at the NSC computer. A first generation of Smart Card login from terminals was developed by a small company (NordNet) in Linköping. The price of a supercomputer was astronomic by today's level. The 2nd hand price for the Cray X-MP/48 was about 60 million SEK. Today any good workstation would do most of the job.

NSC got a quick start with about 200 academic users from all major Swedish universities already the first year. There was quite a broad spectrum of applications such as computational fluid dynamics, condensed matter physics, ecological modelling, geology, mathematics, medical physics, molecular dynamics, numerical combustion, plasma physics, semiconductor devices, statistical physics, structural analysis, and, of course quantum chemistry (as always well prepared and hungry for more flops). There were also industrial users, predominantly from Saab Scania AB because of the company's involvement in NSC. Problem areas were aerodynamics, structural mechanics and electro-magnetic effects. NSC has been quite unique in its close collaborations with Swedish industry, especially with our partners Saab and SMHI. This has contributed fruitfully to the development of NSC over the years.

The Cray X-MP/48 served exceedingly well with great uptime. Scientific demands grow rapidly, however, because of the experience already gained in different fields. Because of this, technological developments and economic realities the Cray X-XMP/48 was replaced in 1993 with a sequence of high-performance computers with a crossover from shared memory vector machines to large computer clusters and, more recently, grid computing and large-scale storage facilities. The tremendous development is illustrated by the figure below with the major NSC resources pictured.

The first 20 years have been interesting and challenging, and it can be expected that the upcoming 20 years will be equally fascinating. There are a lot of challenges ahead, such as growing energy consumption and needs to condense computer systems. Supercomputing will also enter many more scientific fields. In recent years we have seen increased needs in the life science and visualisation areas, and the upcoming demands in life sciences are huge when unravelling the secrets of biological phenomena.

NSC would not have been what it is today if it had not been for all contributions by its devoted staff including preceding directors and all interested users providing important input and essential feedback. It is our vision that NSC will continue to be a leading provider of a wide range of high performance computing services to academic users all over Sweden and our partners Saab AB and SMHI. We will also extend our application expertise and code optimisation staff, which will turn NSC into a more general e-science enabler ready for future challenges in all scientific areas.

KARL-FREDRIK BERGGREN
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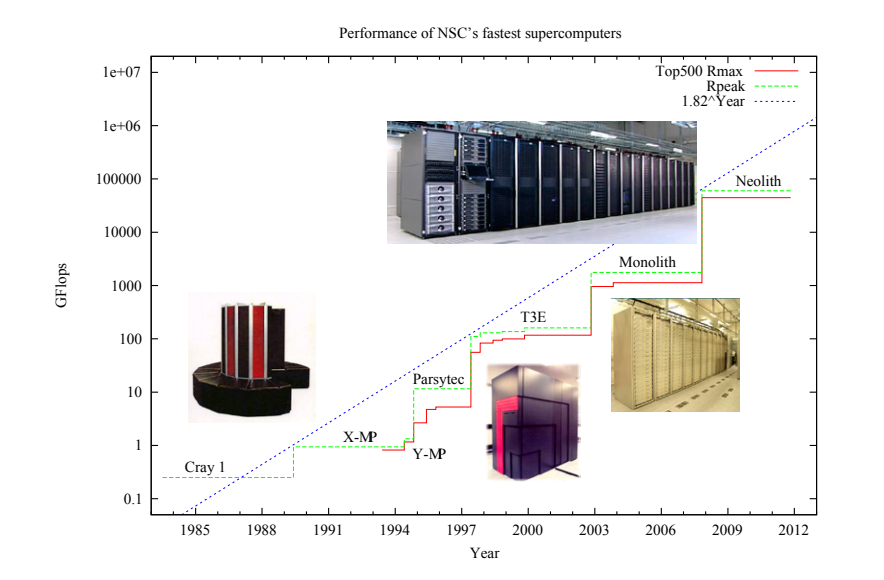

Computational Materials Science fron

The rise in computing power in combination with highly efficient implementations of state-of-the-art theoretical methods makes it possible for computational materials scientists to tackle more and more complex systems at an hitherto unparalleled level of detail. The activities in the Condensed Matter Theory Group of Professor Rajeev Ahuja at the Department of Physics and Materials Science of Uppsala University provide a good example of what breadth of research topics can be investigated nowadays. In the following overview, we describe some of the materials studied by us in greater detail.

Electronic transport on a nanoscale level is a topic of enormous interest these days. Gold nanowires are a particularly attractive target for theoretical studies, and we have demonstrated that the current through gold nanowires can be effectively controlled by stretching or compressing them. Our quantum-mechanical simulations for wires suspended between Au-electrodes reveal that the change in the wire structure induced by pulling apart or pushing together can significantly alter the conductance of the wire. We calculated the conductance of monoatomic Au wires containing 3 – 7 gold atoms from ab initio [1] and found that the transmission depends significantly on the wire stretching and the number of incorporated atoms in good correlation with experiments. Such oscillations are determined by the electronic structure of the one-dimensional part of the wire between the contacts. By pulling the electrodes apart one can make the transmission peak move across the Fermi level, thus modifying the conductance at low bias, an effect which becomes crucial for systems with narrow transmission resonances.

Besides gold nanowires, many other nanoscale materials are discussed for applications in next-generation electronic devices, and graphene is of course a material intensely studied these days. However, a big hurdle for graphene to be a useful electronic material is its lack of an energy gap. We found that Stone-Wales defects break the symmetry enough to induce an opening of an energy gap in the graphene layer(s) above a SiC surface. As the thickness of the graphene layers increases, the energy gap gets smaller. Our results explain observations from recent experiments and suggest a promising approach for band gap engineering in graphene via defects [2].

If a graphene sheet is rolled up, one gets a carbon nanotube (CNT), but in practice one needs to grow CNTs usually through catalytic chemical vapour deposition technique. In order to understand the growth mechanism, molecular dynamics simulations have been used in the temperature range from 800 – 1400 K and it was found that the carbon-metal adhesion strength is crucial for the successful growth of single-walled CNTs. More recently, we were able to determine the adhesion between the metal clusters and CNTs more accurately and found that Fe, Co and Ni, commonly used to catalyse CNT, possess larger adhesion strengths to SWNT than Cu, Pd and Au, and are therefore likely to be more efficient for supporting growth [3].

CNTs can be used in a variety of ways, e.g., even as catalysts for H-storage materials. In a synergistic approach involving experiment and first-principles theory we were able to explain how CNTs and other carbon nanostructures (such as fullerenes) can catalyse the hydrogen uptake and release reactions in complex metal hydrides [4]. Our study was focused on the most widely studied hydrogen storage material, sodium alanate ($NaAlH_4$). The interaction with the electronegative carbon nanostructure substrate affects the ability of Na to donate its charge to AlH_4, consequently weakening the Al-H bond and causing hydrogen to desorb at lower temperatures. In addition, the time evolution of the charge transfer process was revealed from ab initio molecular dynamics simulations.

Staying on the topic of hydrogen storage in metal hydrides, nanostructured MgH_2 can absorb up to 7.7 weight % of hydrogen. Again, one requires a cata-

Crucial Materials Science Challenge Solved

Peter Oppeneer and colleagues have explained the hitherto unsolved mystery in materials science known as 'the hidden order' – how a new phase arises and why. This discovery can be of great importance to our understanding of how new material properties occur, how they can be controlled and exploited in the future.

For a long time researchers have attempted to develop the superconducting materials of the future that will be able to conduct energy without energy losses. The explanation of how a new phase arises can, among other applications, be used for development of new superconducting materials and thus be of importance to future energy supply.

Oppeneer and coworkers have performed large-scale computer calculations, to a large extent on NSC resources, to show how the 'hidden order' emerges. Extremely small magnetic fluctuations prompt changes in the macroscopic properties of the material, so an entirely new phase arises, with different properties.

Their work is published in the scientific journal Nature Materials.

PETER MÜNGER

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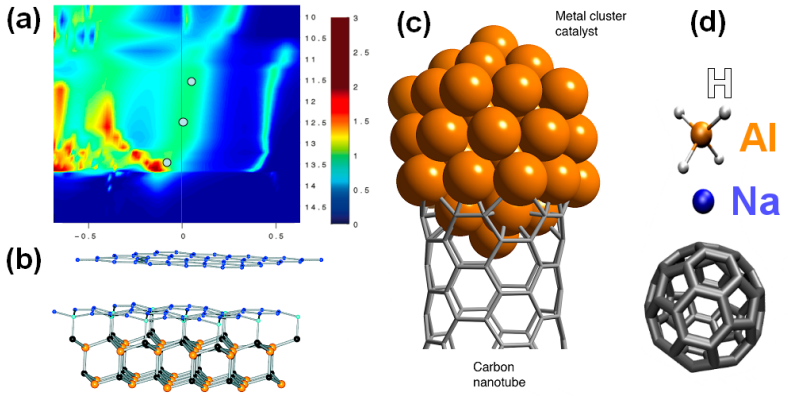

Figure 1: (a) transmission through Au-nanowires plotted on the energy-length plane; (b) graphene layer with Stone-Wales defects on C-SiC with buffer layer; (c) metal cluster and carbon nanotube; (d) sodium alanate interacting with C60 buckyball.

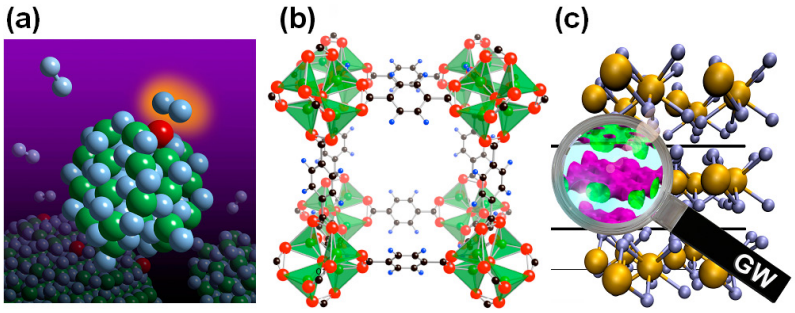

Figure 2: (a) schematic display of a MgH_2 nanocluster with catalyst in the process of hydrogen desorption; (b) MOF-5 showing organic linkers joining metal-oxide clusters; (c) the identified structure of metallic silane with its Fermi surface displayed inside the magnifying glass (the metallic state was confirmed through GW calculations).

lyst to speed up the desorption process, and adding Fe and Ni can be used for this purpose. It has been speculated that the catalysts act as shuttles, helping to transport hydrogen out of the material. We have employed computer simulations of magnesium hydride clusters to understand how this happens and why only a small amount of catalysts are necessary to improve the hydrogen release [5]. Our findings are expected to aid further technical improvements of magnesium-based H-storage materials, as well as other related light metal hydrides.

A completely different class of nanoporous materials discussed for applications in H-storage is formed by metal-organic frameworks (MOFs), which are attractive because the hydrogen sorption process displays good reversibility and fast kinetics in these systems. However, the weak dispersive interactions that hold H_2 molecules require low operations temperatures and/or high pressures. We have studied in particular MOF-5 which consists of 1,4-benzenedicarboxylate linkers joining Zn_4O clusters to form a periodic cubic framework. Our quantum mechanical calculations show [6] that the adsorption of lithium atoms on the organic linkers will greatly increase the strength of the H_2 molecule binding to the framework including electrostatic interactions in addition to the weak dispersive interactions, increasing the temperature at which hydrogen can be stored in MOFs. This discovery makes MOFs more suitable for being used as H-storage materials.

Staying with hydrogen for the last system to be discussed here, silane (SiH_4) is a hydrogen-rich material which can become metallic when sufficiently pressurized. Thus, it provides an interesting opportunity to indirectly study metallic hydrogen and may even provide a pathway to high-temperature superconductivity in hydrogen. Experimentalists have reported on the metallization of silane under pressure,

Large-scale Cluster to NSC

Knut and Alice Wallenberg Foundation has recently granted 14 million SEK to a consortium of Igor Abrikosov and Sven Stafström at Linköping University and researchers at Uppsala University and Royal Institute of Technology for a large-scale computer cluster, dedicated to materials science research. The consortium has an ambitious research program to study new materials for clean energy production and energy storage, new materials and phenomena for energy saving and for hydrogen production and emission reduction, and materials issues of nuclear waste disposal. Even though this is a very broad set of problems, they all rely on a common core of mathematical modeling, mathematical/numerical methods, and simulations. This allows the consortium to efficiently use essentially the same hardware, suitable for solving large linear algebra problems. The new cluster will be equipped with large memory nodes, necessary for the proposed calculations, which is presently not available at any SNIC centre. NSC is very proud to host this new front-line research resource.

BENGT PERSSON

but it remained unclear in what crystal structure silane existed in these experiments. We carried out a systematic theoretical study [7] to determine the structure for metallic silane, and succeeded in identifying one crystal structure from a pool of plausible candidates that matches all requirements. The findings are in excellent agreement with experiment and allowed even for the prediction that the metallic phase of silane could exist at lower pressures.

RAJEEV AHUJA

References

[1] A. Grigoriev, N. V. Skorodumova, S. I. Simak, G. Wendin, B. Johansson and R. Ahuja, Electron transport in stretched monoatomic gold wires, Phys. Rev. Lett. 97, 236807 (2006).
[2] X. Peng and R. Ahuja, Symmetry Breaking Induced Bandgap in Epitaxial Graphene Layers on SiC, Nano Lett. 8, 4464 (2008).
[3] F. Ding, P. Larsson, J. A. Larsson, R. Ahuja, H. Duan, A. Rosen and K. Bolton, The importance of strong carbon-metal adhesion for catalytic nucleation of single-walled carbon nanotubes, Nano Lett. 8, 463 (2008).
[4] P. A. Berseth, A. G. Harter, R. Zidan, A. Blomqvist, C. M. Araújo, R. H. Scheicher, R. Ahuja and P. Jena, Carbon Nanomaterials as Catalysts for Hydrogen Uptake and Release in NaAlH4, Nano Lett. (published online: http://pubs.acs.org/doi/abs/10.1021/nl803498e).
[5] P. Larsson, C. M. Araújo, J. A. Larsson, P. Jena and R. Ahuja, Role of catalysts in dehydrogenation of MgH2 nanoclusters, Proc. Natl. Acad. Sci. USA 105, 8227 (2008).
[6] A. Blomqvist, C. M. Araújo, P. Srepusharawoot and R. Ahuja, Li-decorated metal-organic framework 5: A route to achieving a suitable hydrogen storage medium, Proc. Natl. Acad. Sci. USA 104, 20173 (2007).
[7] D. Y. Kim, R. H. Scheicher, S. Lebègue, J. Prasongkit, B. Arnaud, M. Alouani and R. Ahuja, Crystal structure of the pressure-induced metallic phase of SiH4 from ab initio theory, Proc. Natl. Acad. Sci. USA 105, 16454 (2008).

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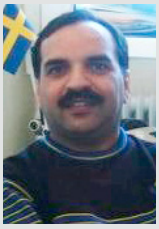

SNIC Storage Group

In 2008, a storage group was formed within SNIC. It is intended to act as a link between the centres and as an expert group in relation to the SNIC board and to SNAC. It should also be involved in discussions and cooperations between SNIC and other parties in matters concerning storage. The group is composed of one representative from each centre and the SweGrid coordinator.

One of the main tasks of the storage group is to plan and follow up on the implementation of the storage infrastructure of SNIC and the associated services. According to the strategy prepared by the group, this infrastructure should contain nationally accessible storage and centre storage, which, when implemented, will represent two new types of services.

Nationally accessible storage is intended for projects that need to reach their data from different places, e.g., different centres, and for long-term storage. This storage should not only be available to the traditional users within SNIC, i.e., computationally intensive projects, but also to other groups. A national language database has already been offered disk space, ready to be incorporated into the nationally accessible storage solution when it is operational.

Centre storage should be available at each SNIC centre and have a life of its own independent of the cluster resources; i.e., there should be a long-term commitment from SNIC to maintain a continuously renewable and expandable storage solution at each centre. Today, storage is usually tied to a cluster with a limited lifespan. There will still be cluster-specific storage in the future, to offer the best performance, but centre storage is needed to facilitate data management and create continuity.

Harmonisation of the user environments at the centres is another issue. Todays solutions have grown out of different traditions at the centres. The storage group is presently working to establish guidelines and common elements that will allow the users to use the same approach to handling data at different centres.

On the international level, a cooperation with NOTUR, SNICs Norwegian counterpart, and its storage project NorStore is in the making. Sweden and the other Nordic countries are also involved in a cooperation regarding LHC data within NDGF. Currently, this cooperation is coordinated through SweGrid. This is expected to lead to both synergies and valueable experiences that may be used, e.g., when setting up nationally accessible storage.

Nationally, close cooperation is expected with other organisations within the Swedish Research Council, e.g., DISC. Here SNIC can contribute technical expertise in the creation of a storage infrastructure. An example of cooperation within SNIC is that centres without tape backup of their own may use tape backup existing at other centres.

TOM LANGBORG

UPCOMING EVENTS

DEISA PRACE Symposium 2009: HPC Infrastructures for Petascale Applications
May 11 – 13, 2009, Amsterdam, The Netherlands.
http://www.prace-project.eu/events/prace-deisa-scientific-conference-may-2009-amsterdam-the-netherlands

ACM International Conference on Computing Frontiers
May 18 – 20, 2009, Ischia, Italy.
http://www.computingfrontiers.org/2009

CCGrid09; 9th IEEE International Symposium on Cluster Computing and the Grid
May 18 – 21, 2009, Shanghai, China.
http://grid.sjtu.edu.cn/ccgrid2009

IPDPS-09: IEEE International Parallel and Distributed Processing Symposium
May 25 – 29, 2009, Rome, Italy.
http://ipdps.org

HiCOMB 2009 8th IEEE International Workshop on High Performance Computational Biology
May 25, 2009, Rome, Italy.
http://www.hicomb.org

ICS'09: 23rd International Conference on Supercomputing
June 9 – 11, 2009, New York, USA.
http://www.ics-conference.org

HPDC 2009; International Symposium on High Performance Distributed Computing
June 11 – 13, 2009, Munich, Germany.
http://www.lrz-muenchen.de/hpdc2009

ISC'09: International Supercomputing Conference
June 23 – 26, 2009, Hamburg, Germany.
http://www.isc09.org

Euro-Par 2009; European Conference on Parallel Computing
August 25 – 28, 2009, Delft, The Netherlands.
http://europar2009.ewi.tudelft.nl

IEEE Cluster 2009
August 31 – Sept. 4, 2009, New Orleans, Louisiana, USA.
http://www.cluster2009.org

ParCo2009; International Conference on Parallel Computing
September 1 – 4, 2009, Lyon, France.
http://www.ens-lyon.fr/LIP/ParCo09-3

PACT2009; The 18th International Conference on Parallel Architectures and Compilation Techniques
September 12 – 16, 2009, Raleigh, North Carolina, USA.
http://www.pactconf.org

ICPP-2009; 38th International Conference on Parallel Processsssing
September 22 – 25, 2009, Vienna, Austria.
http://www.cse.ohio-state.edu/~icpp2009

SC09; International Conference for High Performance Computing, Networking, Storage and Analysis
November 14 – 20, 2009, Portland, Oregon.
http://sc09.supercomputing.org

HiPC 2009; 16th IEEE International Conference on High Performance Computing
December 16 – 19, 2009, Kochi, India
http://www.hipc.org

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