



DEISA deployed for advancing research into behaviour of liquids

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Ari Paavo Seitsonen and his research group have simulated molecular liquids using *ab initio* molecular dynamics methods. The research helps to understand the structures and properties of new environmentally friendly solvents. The project also clarifies how taking dispersion interactions into account affects the electron structure.

The computing resources of the EPCC supercomputing centre in Scotland were used when the AIMDliqD (*Ab Initio* Molecular Dynamics for Liquids and Diamond) project was implemented as part of extensive continuing international collaboration. Molecular dynamics methods were used for simulating two liquids at the atomic level to provide a realistic finite-temperature description.

"In *ab initio* methods the system's electron structure is explicitly solved. Being a dynamic simulation, describing the structure requires solving the electronic structure consecutively many times during the dynamic simulation. This substantially increases the required computation capacity compared with, for example, simulations performed using parameterized potential energy models. However, the attained results are more reliable and usually more accurate", says Ari Paavo Seitsonen, research engineer from the Institute of Mineralogy and Physics at Université Pierre et Marie Curie.

Ab initio-based simulation produces the system's electron structure, while traditional parameterized models only provide positions for the nuclei and the system's total energy. Electronic structure analysis is also useful for investigating other properties of the material and reasons behind them. These properties cannot be investigated using classical or semiempirical methods. *Ab initio* molecular dynamics (AIMD) methods reveal information about the target that might never be gained through other simulations or experimental techniques. It is extremely difficult to conduct empirical studies on, for example, the short-lived hydro-

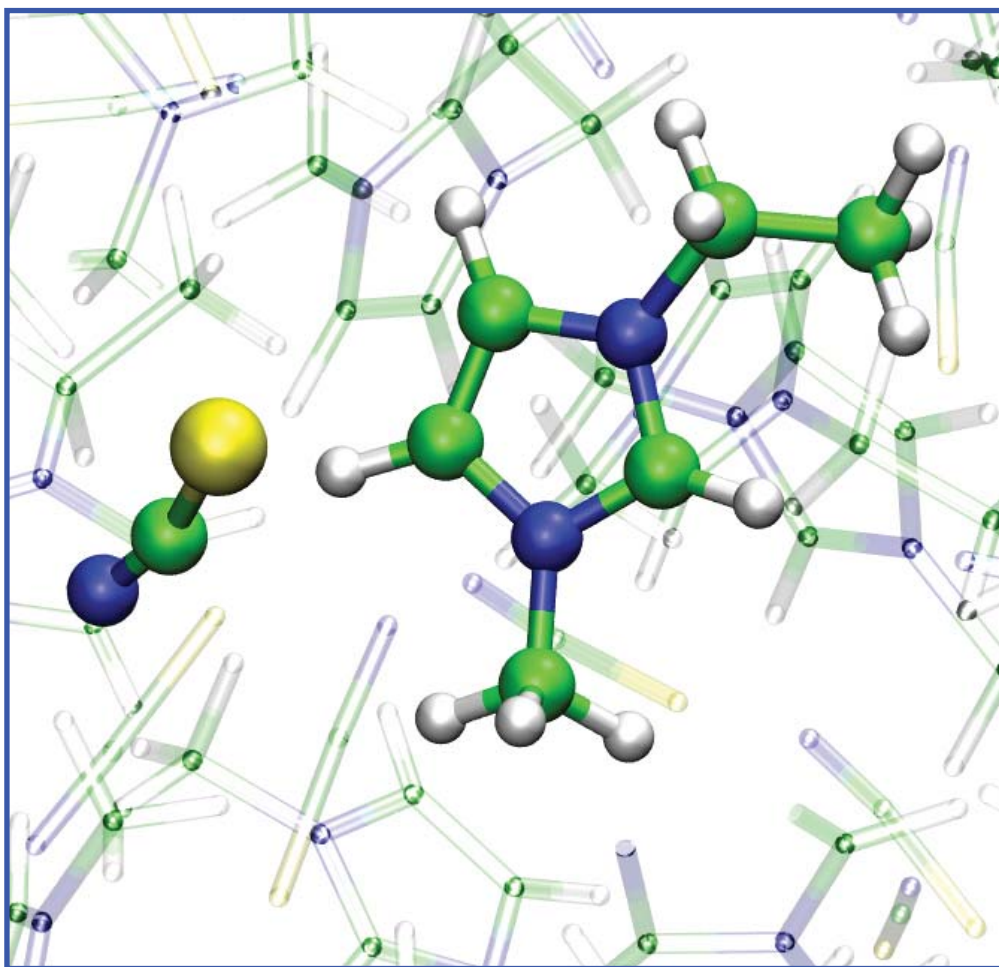


Fig. 1. A snapshot from a molecular dynamics simulation showing one molecular pair of the ionic liquid EMIM-SCN. Yellow stands for sulfur, green for carbon, blue for nitrogen, and white for hydrogen

gen bonds or other contacts and short-distance range structures in a liquid. Yet these have a significant effect on, for example, solvents' functions. Over the past few years, parameterized energy potentials have been used in several simulations. The results gained in the AIMDliqD project can also be used for evaluating the accuracy of these simulations.

One of the biggest simulations ever

Ari Paavo Seitsonen started his current work at the beginning of 2005. He is involved in several collaboration projects with European re-

searchers in the fields of physical chemistry and surface physics.

Seitsonen, as the responsible project leader collaborated in the AIMDliqD project with Professor Barbara Kirchner and her research group at the Wilhelm-Ostwald-Institut, Universität Leipzig, Professor Jürg Hutter's group at the Institute of Physical Chemistry, University of Zurich, and Professor Kari Laasonen's group at the University of Oulu.

The computational simulations for the AIMDliqD project were performed during the spring and early summer of 2007 at EPCC in Scotland. Ari Paavo Seitsonen was mainly re-

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sponsible for the computation, but all groups have participated in the actual project planning and results analyses. The results analyses are still ongoing and once they are completed, several scientific publications will follow.

"The project is part of our continuing international collaboration. These research groups involved have worked together before, especially on ionic liquids, and work will continue, in the form of new projects. Only a few *ab initio* simulations have previously been executed for ionic liquids, and the one performed in the AIMDliqD project was one of the largest", Seitsonen explains, to clarify the significance of the project.

Discovering basic properties of ionic liquids

"In the AIMDliqD project we focused on two targets. The first was the effect of weak forc-

es, van der Waals interactions in particular, on molecular dynamics and consequently, on the properties of the liquids. The second was the ionic liquids, which have become a keen topic of interest in recent years in the field of "green chemistry", says Seitsonen.

To date, very few *ab initio* molecular dynamic simulations have been carried out to investigate the importance of van der Waals forces, because modelling these forces analytically is difficult. Professor Ursula Röthlisberger's group at the EPFL in Lausanne has quite recently developed a computational method that allows the calculation of these forces to be included in the AIMD calculations with only a minor additional computational effort.

"We simulated a liquid using an *ab initio* model with and without the van der Waals forces. The results of these computations enable us to make conclusions on the sig-

nificance of these forces for the material's properties. The van der Waals forces are especially important in interactions between molecules. They are weaker than hydrogen bonding or electrostatic interactions that occur between charges. However, they are the origin of forces such as those keeping hydrocarbons in a liquid state", says Seitsonen.

The increasing interest in ionic liquids is due to the reduced losses during chemical reactions. Ionic liquids can be effectively recycled, so no chemical waste is produced. The diverse properties of ionic liquids also pave the way for energy-efficient or unmatched process conditions superior to those obtainable with traditional solvents. Many of the basic properties of ionic liquids are not completely understood; the AIMDliqD project serves to fulfil this information gap.

Figure 2 shows how electron density in liquid benzene changes, when van der Waals interactions have been taken into account via the method used in this project. The picture reveals that electron density is shifted from the immediate vicinity of atoms (blue) to the intra-molecular space (red). The electron density helps us to understand the attraction forces between molecules.

Massive tools are needed

The computation time allocated to the AIMDliqD project was essential for carrying out the study. The simulations require heavy-duty computation and they must be performed with massively parallel computers. To cope with these requirements, the resources given by DEISA were needed. The simulation of the ionic liquid consisted of 64 ion pairs (1-ethyl-3-methylimidazolium cation EMIM⁺ and thiocyanate anion SCN⁻), i.e. 1048 atoms with 3840 valence electrons to be calculated explicitly.

"For our practical calculations the Unicore Client interface was a very good tool, because it hid the complexities of the grid calculation from the user. Unicore Client is the software that integrates all DEISA centres. Computation jobs are submitted via the Unicore Client to be run by supercomputers in different computing centres. Furthermore, the participants at EPCC also supported us in running our computations, which was important especially at the early phase of the project", says Seitsonen.

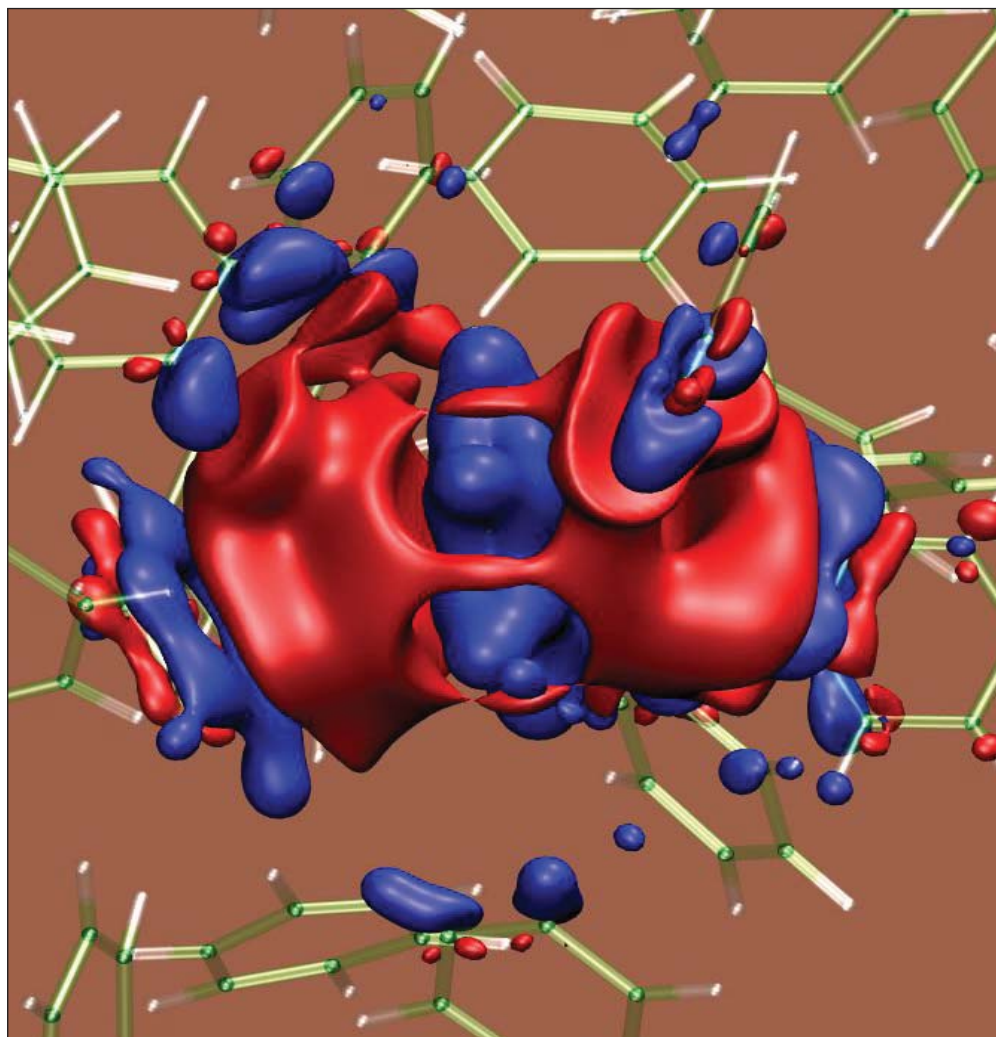


Fig. 2. Change in electron density in liquid benzene due to the van der Waals interactions: Red regions, increased electron density; blue regions, decreased electron density.

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The project belongs to basic research, and it does not have direct applications. Usually, temperature is not directly taken into account at the atomic level when reaction barriers are being studied; its effect is calculated afterwards using different approximations. This can comprise a serious flaw, if the solvent participates in the chemical reactions or if it plays a major role in another way. This can be avoided by using *ab initio* molecular dynamic methods. An aim for the future is to be able to simulate also industrially relevant chemical reactions in ionic liquids. Hence, simulations such as those in the AIMDliqD project could be used to introduce quantitative analyses for studying reaction barriers and processes.



Fig. 3. Ari Paavo Seitsonen, research engineer from the Institute of Mineralogy and Physics at Université Pierre et Marie Curie

DEISA Extreme Computing Initiative Call for Proposals 2009

Identifier: DECI-5

Closing date: May 4, 2009

The DEISA Extreme Computing Initiative (DECI) is a scheme through which European computational scientists can apply for single-project access to world-leading computational resources in the European HPC infrastructure, operated by DEISA, for a period of up to 12 months. DECI aims to enable European researchers to obtain access to the most powerful national computing resources in Europe, regardless of their country of origin or work and to enhance DEISA's impact on European science and technology at the highest level.

Through an open, competitive call, a number of capability computing projects will be selected on the basis of innovation and scientific excellence. These projects must deal with complex, demanding, innovative simulations that would not be possible without the DEISA infrastructure, and which would benefit from the exceptional resources of the Consortium. In addition to offering access to computing resources, DEISA offers applications-enabling assistance from experts at the leading European HPC centres to enable projects to be run on the most appropriate platforms in the DEISA consortium.

Projects supported by DECI will be chosen on the basis of innovation potential, scientific excellence and relevance criteria. Priority will be given to proposals that promote collaborative research, either at a cross-national or cross-disciplinary level. Further, proposals from PIs that have yet to benefit from DECI compute and applications enabling resources may be given preference. Proposals selected under this call will be given access to the infrastructure for applications enabling from 1 October 2009 and for production runs from 1 November 2009 to 30 September 2010.

Applications profiles supported by DECI

The following applications profiles are particularly suited to the DECI:

- Large, highly scalable parallel applications requiring exceptional computational resources
- Data intensive applications requiring access to distributed data repositories
- Workflow Simulations managing simulation chains that access more than one computing platform
- Distributed applications that need to run on more than one platform (excluding meta-computing)

DEISA can provide applications enabling support (typically up to several months) for the enabling and optimisation of these applications.

Support for the Initiative

In order to facilitate the identification and the support of leading applications for the DEISA infrastructure, the Consortium has set up an 'Applications Task Force' (ATASKF) comprising experts in high performance and Grid computing from each of the DEISA member organisations. Scientists interested in responding to the call, or in finding out more about what DECI and the DEISA infrastructure can offer them, should contact the Applications Task Force for advice on finding the best fit between their requirements and the DEISA distributed supercomputing environment.

Call for proposals

To answer to the call, please see more details at: www.deisa.eu/science/deci/deci-call-for-proposals2009

Successful UNICORE and Supercomputing Workshop 2009

On March 18, 2009 the UNICORE and Supercomputing Workshop took place at the Deutscher Wetterdienst (DWD) in Offenbach near Frankfurt, Germany. The objective of the workshop was

to present and demonstrate interesting results of UNICORE usage in Supercomputing to major stakeholders in Supercomputing from Germany and Europe as well as to members of the UNICORE Forum (www.unicore.eu/forum). About 40 people participated in the workshop and listened to the seven speakers. The workshop opened with an overview on UNICORE 6 followed by presentations from the life-science

domain, the exploitation of DEISA – the European Supercomputing Grid e-infrastructure – and presentations from the French Atomic Energy Commission CEA and T-Systems SfR about the usage and adaptation of UNICORE in industrial environments. The detailed program and all presentations as PDF can be found at: www.unicore.eu/events/supercomputing-workshop-2009

Metal adsorption on nanostructured ultrathin films

Giovanni Barcaro and Alessandro Fortunelli, IPCF-CNR, Pisa, Italy
Paolo Giannozzi, University of Udine, Italy

This project shows that the use of supercomputing facilities allows one to predict structure and properties of nanostructured ultrathin films, fully clarifying unresolved experimental issues.

Metal adsorption on two nanostructured titania (TiO_x) ultrathin films grown on the Pt(111) surface is investigated via a first-principles computational approach. These films present very regular nanopatterns extending over mesoscopic distances, with compact regions intercalated by point defects which act as nucleation and trapping centers, and are thus of great interest as nanotemplates for the growth of ordered supra-assemblies of equally sized (monodisperse) metal nanoclusters. However, due to the large size of their unit cells, their theoretical investigation has been so far hindered by computational limitations.

Our study shows that the use of supercomputing facilities, like those made available through the DEISA initiative, allows one to predict structure and properties of these systems, fully clarifying unresolved experimental issues such as a metal-induced phase transformation. The obtained results are also discussed as paradigmatic examples of the interaction of metals with polar ultrathin films of oxides grown on metal supports, a novel and promising field in materials science.

Metal on oxide on metal

Metal clusters adsorbed on oxide surfaces are the subject of considerable attention due to their scientific interest and technological applications, and this has fuelled a series of fundamental studies on model systems obtained by metal deposition on oxide single crystals in UHV. More recently, attention has shifted from single crystals to ultrathin films grown on metal supports, as they allow STM measurements to be performed. The underlying metal support can, however, actively participate in the adsorption process, producing a wealth of novel phenomena and posing new issues and challenges. In this field, oxide *polar* nanophases represent a pioneering and even less unexplored topic, particularly promising for their templating characteristics. Computational approaches are expected to play an impor-

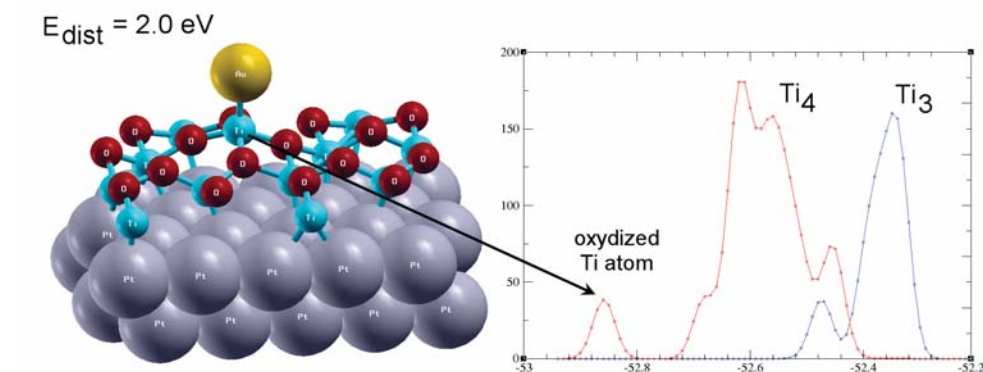


Fig. 4. Surface reconstruction (left) after the adsorption of a gold atom on the z' - $\text{TiO}_x/\text{Pt}(111)$ phase (gold, titanium, oxygen and platinum as yellow, light blue, red and grey, respectively) and Density of States (PDOS, right) projected on the Ti 3s (semi-core) states. The PDOS of the Ti atom interacting with adsorbed gold appears as a peak shifted at higher binding energies

tant role in the study of these systems, but their application is limited by the large size of the unit cells. In the present study we focused on two such oxide polar ultrathin phases, namely the z - and z' - TiO_x (titania) phases grown on the Pt(111) surface exhibiting a zig-zag-like habitus in their STM images, and we investigated via a first-principles approach the characteristics of metal adsorption on them. The $\text{TiO}_x/\text{Pt}(111)$ system is chosen as it presents a variety of phases with different topographies providing a fairly complete representation of the various possibilities, while the dimensions of the unit cells allow one to perform systematic investigations.

Computational approach

We used state-of-the-art first-principles electronic-structure techniques to investigate the structure of the titania films and metal adsorption on them. In particular, we used two plane-wave codes: PWscf for energy minimizations and wave function analysis, and CP (Car-Parinello) for dynamics simulations, both taken from the ESPRESSO software package. The calculations, totalling 350,000 CPU-hours, were carried out at the Louhi (Cray XT4) supercomputer of CSC in Espoo, Finland.

The project was mainly articulated in two steps: (1) potential energy landscape for the adsorption of single metal atoms; (2) small cluster epitaxy and influence of metal adsorption on the structure of the films.

Adsorption of single metal atoms

After confirming previous structural assignments via dynamic (CP) simulations on the bare titania phases, the first step of the project consisted in exploring the potential energy surface for the adsorption of single metal atoms. Au, Pd and Fe atoms were selected as prototypical examples. A very different landscape was found to occur as a function of the electron affinity and the chemical properties of the adsorbed metal atom, with a peculiar surface reconstruction induced by a Au atom (see figure).

Adsorption of metal clusters

Calculations were made in two steps. First, density-functional global optimization (DF-GO) calculations were performed to elucidate the structure, epitaxy and energetics of adsorbed Au clusters. This was the first time that DF-GO calculations were performed on systems of this size and corresponded to the most computationally intensive part of the project. The simulated STM images of cluster growth were in agreement with experimental results. Then, the influence of the metal adsorption on the structure of the z' -film was studied as a function of temperature. It was found that Au (but *not*, e.g., Fe) induces a surface reconstruction from a rectangular to a hexagonal phase (one of the first examples of a metal- and heat-induced phase transformation in oxide nanophases). This metal-induced phase transformation was proved to be favourable at both the static (DF-GO) and dynamic (CP) level.

DEISA PRACE Symposium 2009

“HPC Infrastructures for Petascale Applications”

11-13 May, 2009, Amsterdam



PRELIMINARY PROGRAMME

Monday, May 11 (12:00 – 18:00)

12:00 Registration and lunch in the
Royal Tropical Institute

13:00 Welcome

“Global Perspectives 1”

Mario Campolargo, EU
Ed Seidel, NSF, US
Ryutaro Himeno, RIKEN, JP
Ben Evans, ANU-SF, Australia
Horst Simon, DoE, NERSC, US

Tuesday, May 12 (9:00 – 18:00)

“Global Perspectives 2”

Kostas Glinos, EU
Achim Bachem, PRACE
Stefan Heinzel, DEISA
John Towns, TeraGrid, US

“Science Communities”

Climate Research: Sylvie Joussaume, France
Cosmology: Carlos Frenk, UK
Fusion Research: Frank Jenko, DE
Life Sciences: Peter Coveney, UK

“PRACE Perspectives”

Directions in HPC Technology: Jean-Marie
Normand, CEA
Survey of HPC Systems and Applications in
Europe: Mark Bull, EPCC
Training and Education for Petascale Computing:
Tim Stitt, CSCS

“DEISA Extreme Computing 1”

Speakers from different areas of science from
all over Europe

Evening Conference Dinner

Wednesday, May 13 (9:00 – 13:00)

“DEISA Extreme Computing 2”

Speakers from different areas of science from
all over Europe

Closing remarks

13:00 Lunch

Registration and more information:
http://www.deisa.eu/news_press/symposium

Contact information:
deisa-prace-symposium-contact@fz-juelich.de