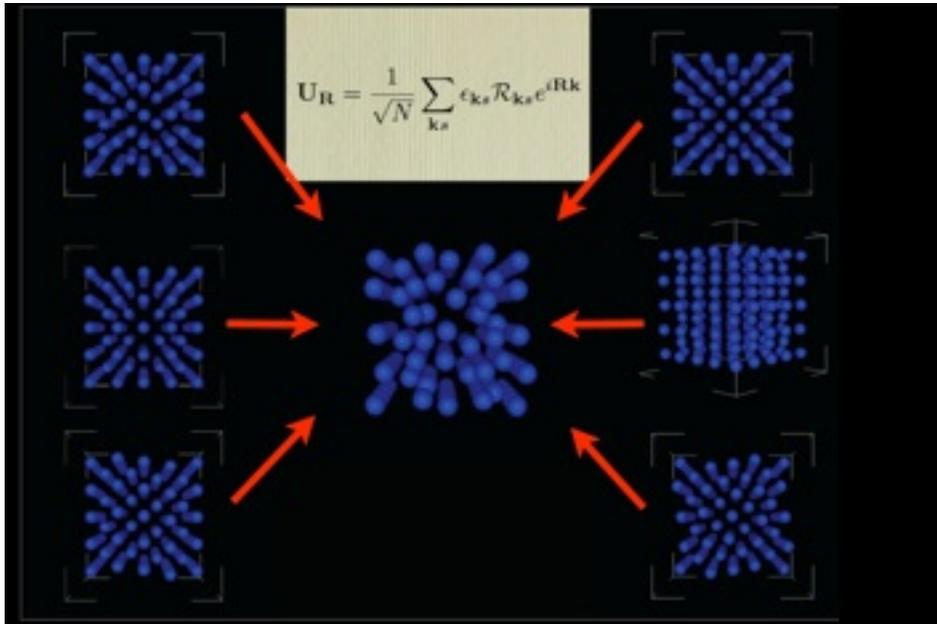


WORKSHOP ON THE SCAILD METHOD AND  
SIMILAR COMPUTATIONAL APPROCHES IN

LATTICE DYNAMICS

27-28 AUGUST 2012 IN UPPSALA



Organized by Uppsala University

Initiative of Université de Liège

# TENTATIVE WORKSHOP PROGRAM:

## Monday the 27 August:

**10:30-10:45** Welcoming the Participants of the Workshop and some communication of basic information concerning practicalities.

Short introductory presentations of the SCAILD method:

**10:50-11:05 Past, present and future of the SCAILD type of methodology.** By Petros Souvatzis, Uppsala University

**11:10-11:30 The self-consistent ab-initio lattice dynamical method interfaced with ABINIT and Quantum Espresso.** By Dr. Srijan Kumar Saha, Universite de Liege.

**11:35-11:55 Implementation of the SCAILD method within the ELK framework.** By Prof. Dr. Aldo Humberto Romero, Max Planck Institute, fuer Mikrostrukturre Physik, Halle.

**12:00-13:00 LUNCH**

**13:00-13:20 Something by Matthieu Verstraete ?**

**13:25-13:45 Anharmonicity and the stability of the simple cubic phase of calcium** , by Marco Di Gennaro, Universite de Liege.

Alternative methods of including anharmonic effects from first principles:

**13:50-14:10 FINITE TEMPERATURE EFFECTS IN *AB INITIO* SIMULATIONS OF MATERIALS PROPERTIES (Activities at Linköping University, Part I)** , by Professor Igor A. Abrikosov , Linköping University.

**14:15-14:35 FINITE TEMPERATURE EFFECTS IN *AB INITIO* SIMULATIONS OF MATERIALS PROPERTIES (Activities at Linköping University, Part II)** , by Olle Hellman, Linköping University.

Some recent preliminary results obtained with the scaild methodology:

**14:40-15:00 Dynamic Stabilization of cubic AuZn by means of phonon-phonon interaction.** By Leyla Isaeva, Uppsala University.

**15:05 COFFE BREAK**

**15:20-15:40 Something by Baotian Wang. Sb<sub>2</sub>Te<sub>3</sub> or bcc/hcp Fe ?**

**15:45-17:00 Open discussion concerning:**

(1) comparison with the half dozen other Born/SCphonon-type methods which appeared since scaild, about generality, convergence, etc...

(2) Doing the stochastic steps in a Monte Carlo way instead of random displacements as a function of Q and T etc...

(3) Supercell size convergence

(4) Dielectric effects - limitations of Parlinskii and other methods

**19:00 DINNER**

**Tuesday the 27 August:**

Results of softmode materials studied with conventional lattice dynamical methods:

**09:00-09:20 Soft modes in strained and unstrained rutile TiO<sub>2</sub>.** By Pavlin Mitev, Uppsala University

**09:25-09:45 Free for presentation.**

**09:50-10:10 Free for presentation.**

**10:15-10:30 COFFE BREAK**

**10:30-10:50 Free for presentation.**

**10:55-12:00 Closing discussion.**

**Practical Information:**

The workshop will take place in the bottom floor of the Ångström laboratory in room **80121** see attached map in the end of this pdf. Also, you will find information on how to get to the Ångström laboratory from the city center of Uppsala.

## Abstracts:

Title : **The self-consistent ab-initio lattice dynamical method interfaced with ABINIT and Quantum Espresso**

Speaker : Dr. Srijan Kumar Saha

Abstract :

Conventional methods to calculate the thermodynamical properties of crystals use the harmonic phonon spectra and hence, do not work in the case where the studied crystal structure exhibits unstable phonon modes at zero Kelvin; this is, for instance, the case in the high temperature body-centered cubic (bcc) phase of many metals or the high-temperature phases of ferroelectric compounds. To calculate temperature dependent phonon spectra, recently (PRL 100, 095901, 2008), the self-consistent ab-initio lattice dynamical (SCAILD) method has been developed. This method is being implemented in ABINIT package. In order to benchmark this on-going development, I interface the SCAILD code with the ABINIT and Quantum-Espresso package. Our results for temperature dependent phonon spectra of ABX3 functional materials will be discussed.

## **FINITE TEMPERATURE EFFECTS IN *AB INITIO* SIMULATIONS OF MATERIALS PROPERTIES**

Olle Hellman, Peter Steneteg, Björn Alling, Olga Yu. Vekilova, Nina Shulumba,

Ferenc Tasnadi, Sergei I. Simak, and Igor A. Abrikosov

*Department of Physics, Chemistry and Biology, Linköping University, Sweden.*

*Ab initio* electronic structure theory is known as a useful tool for prediction of materials properties, for their understanding, as well as for determination of parameters employed in higher-level modeling. However, majority of simulations still deal with calculations in the framework of density functional theory (DFT) with local or semi-local functionals carried out at zero temperature. In this talk we present new methodological solutions, which go beyond this approach and explicitly take finite temperature effects into account.

In particular, an accurate and easily extendable method to deal with lattice dynamics of solids is offered [1]. It is based on *ab initio* molecular dynamics (AIMD) simulations and provides a consistent way to extract the best possible harmonic—or higher order—potential energy surface at finite temperatures. It is designed to work even for strongly anharmonic systems where the traditional quasiharmonic approximation fails. The accuracy and convergence of the method are controlled in a straightforward way. Excellent agreement of the calculated phonon dispersion relations at finite temperature and pressure-temperature phase diagram with experimental results for bcc Zr is demonstrated.

Next, we suggest first-principles method for the calculation of thermodynamic properties of magnetic materials in their high-temperature paramagnetic phase [2]. It is based on AIMD and simultaneous redistributions of the disordered but finite local magnetic moments. We apply this disordered local moments molecular dynamics method to simulate equation of state of CrN, and show that when magnetic disorder and strong electron correlations are taken into account simultaneously, pressure- and temperature-induced structural and magnetic transitions in CrN can be understood [2,3].

Finally, we study elastic properties of TiN within a wide temperature interval [4]. Computational efficiency of the method is greatly enhanced by a careful preparation of the initial state of the simulation cell that allows for a parallel implementation of AIMD calculations. Single crystal elastic constants  $C_{11}$ ,  $C_{12}$  and  $C_{44}$  are calculated. In all cases strong dependence on the temperature is predicted, with  $C_{11}$  decreasing by more than 30% at 1800 K as compared to its value obtained in conventional static calculations at  $T=0\text{K}$ . We observe that the material becomes substantially more isotropic at high temperatures. Our results unambiguously demonstrate importance of taking into account finite temperature effects in theoretical calculations of thermodynamic and elastic properties of materials.

[1] O. Hellman, I. A. Abrikosov, and S. I. Simak, Phys. Rev. B **84**, 180301(R) (2011).

[2] P. Steneteg, B. Alling, I. A. Abrikosov, Phys. Rev. B **85**, 144404 (2012).

[3] B. Alling, T. Marten, and I. A. Abrikosov, Nature Materials **9**, (2010) 283; B. Alling, T. Marten, and I. A. Abrikosov, Phys. Rev. B **82**, (2010) 184430.

[4] P. Steneteg, O. Hellman, O. Yu. Vekilova, N. Shulumba, F. Tasnadi, and I. A. Abrikosov, in manuscript.

# Dynamic stabilization of cubic AuZn by means of phonon-phonon interaction

Leyla Isaeva, Petros Souvatzis, Olle Eriksson

*Division of Materials Theory, Department of Physics and Astronomy, Uppsala University, SE-751 20 Uppsala, Sweden*

Jason C. Lashley

*Los Alamos National Laboratory, Los Alamos, New Mexico, 87545, USA*

(Dated: July 31, 2012)

We have studied the mechanism of B2→P3 martensitic transformation in the shape memory alloy AuZn using the SCAILD technique. The soft Zener mode along  $\Gamma$ -M direction is shown to be stabilized when taking into account phonon-phonon interaction. The theoretical transformation temperature produced by the SCAILD technique is in favorable agreement with the experiment. Fermi surface topology of B2-AuZn has been studied and it has been shown that the large area of the Fermi surface can be nested with the other areas by translation through the vector  $\mathbf{q} \approx \frac{1}{3}[1, 1, 0]$  that is associated with the softening in vibrational spectrum. First-principles calculations have been performed to study the contribution of the bare-static susceptibility to electron-phonon coupling. We argue that strong electron-phonon coupling can be a driving force for the B2→P3 martensitic transformation in AuZn.

# Anharmonicity and the stability of the simple cubic phase of calcium

Marco Di Gennaro, Srijan K. Saha and Matthieu J. Verstraete<sup>1,\*</sup>

<sup>1</sup>*Department of Physics, Université de Liège, B-4000 Liège, Belgium*

In the 32-109GPa pressure range and at room temperature, a simple cubic phase was observed for Ca in at least 4 experiments, harmonic linear response calculations within density functional theory give dynamical instability. We review the stability of the simple cubic phase of Calcium taking explicitly into account thermal corrections relative to electronic as well as phononic entropy and anharmonic contributions, in order to correct the discrepancies among previous theoretical results and experiments. Transport quantities are calculated to provide additional points of comparison with experiments.

# Soft modes in strained and unstrained rutile TiO<sub>2</sub>

Pavlin D. Mitev<sup>\*,†</sup>, Kersti Hermansson<sup>\*,†</sup>, Barbara Montanari<sup>‡</sup>, and Keith Refson<sup>‡</sup>

<sup>\*</sup>Materials Chemistry, Ångström Laboratory, P.O. Box 538, SE-752 21 Uppsala, Sweden

<sup>†</sup>Theoretical Chemistry, Royal Institute of Technology, SE-100 44 Stockholm, Sweden

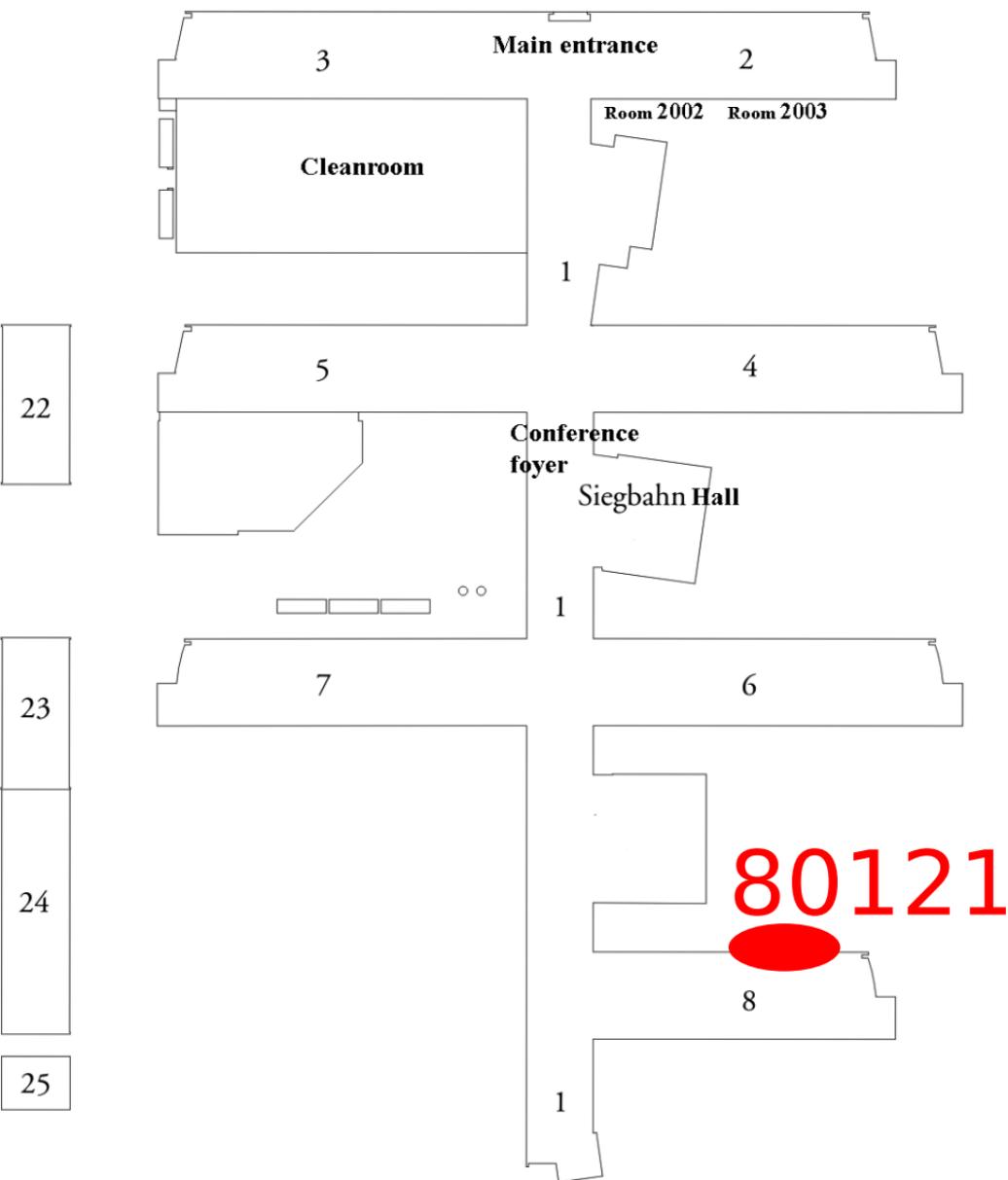
<sup>‡</sup>STFC Rutherford Appleton Laboratory, Chilton, Didcot OX11 0QX, United Kingdom

The lattice dynamics of crystalline TiO<sub>2</sub> was studied using density-functional perturbation theory and the local-density approximation in a plane-wave pseudopotential formalism in equilibrium and uniaxially strained geometries. Here we present well-converged phonon dispersion calculations, which sample a more complete volume of the Brillouin zone than in previous studies. We find an anomalously soft TA mode in a region of reciprocal-space previously unexplored either by any previous calculation or experiment. This is quite independent from the A<sub>2u</sub> mode which becomes soft at the gamma point and is responsible for the incipient ferroelectric behavior. The harmonic frequency of the soft TA mode around  $q=(\frac{1}{2},\frac{1}{2},\frac{1}{4})$  decreases to zero under an isotropic expansion with a strain slightly above 0.5%. In addition to the softening under isotropic strain, the frequency of this mode goes to zero under uniaxial strain along the [110] direction in both compression and expansion (at close to -0.5% and +1.0%, respectively), which offers possibilities for experimental tests of softening under compressional strain. We further suggest that the soft TA mode may help explain the anomalously long-ranged convergence observed in previous calculations on slab models of the TiO<sub>2</sub> [110] surface by providing a mechanism for small changes in bonding at the surface to propagate deep into the bulk. The behavior of other modes under strain was also studied.

## References

1. P.D. Mitev, K. Hermansson, B. Montanari, and K. Refson, Phys. Rev. B, 81, (2010), 134303.

# MAPS AND DIRECTIONS - ÅNGSTRÖM LABORATORY



**Explanation room locations:** Room number 2002 is located in building 2 on floor 0 (ground floor). Room number 12167 is consequently located in building 1, on floor 2 and room 167, and so on.

