# PROPOSAL FOR A WORKSHOP

1.**Workshop title:**

## 2-d WORKSHOP ON *AB INITIO* PHONON CALCULATIONS

2.**Proposed dates and location of the workshop**:

2.5 days, December 2007,
Arrival 5.12.2007 evening, departure 8.12.2007.
Pedagogical University, Cracow, Poland.
(There are also cheap flight conections between many of European airports and Cracow)

3.**Name and full coordinates of applicant:**

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and
Institute of Technics
Pedagogical University, Cracow

4.**Keywords relating to the proposed workshop topic:**

PHONONS DIRECT METHOD
NANOMATERIALS
AB INITIO CALCULATIONS

5.**Abstract of the proposed workshop topic:**

Phonons are the fundamental excitations which represent the elementary vibrations in solid state materials, and to large extend define the materials thermodynamics, and finite temperature properties. They play an important role for quite a number of phenomena mentioning only the thermal expansion, temperature dependence of mechanical properties, phase transitions, and phase diagrams. In surfaces, interfaces, multilayers, crystals with defects and impurities, etc. the role of phonons have not yet been understood completely.

The purpose of the Workshop is to present results of such calculations, make the participants familiar with the numerical tools which allow the *ab initio* phonon computations. There is also possibility to organize the tutorials in the computer rooms.

## 6.**The case for an exploratory workshop:**

Phonons occur everywhere since they manifest the presence of temperature. In crystalline materials such a phononic motion can be quite well classified. Phonons play an important role for quite a number of microscopic and bulk phenomena such as inelastic coherent and incoherent neutron scattering, coherent inelastic X-ray scattering, inelastic nuclear absorption, infrared absorption, raman scattering. Large part of the temperature dependence of the thermodynamic functions comes from phonons. Hence, phonons influence the phase diagrams, chemical reactions, atomic diffusion, thermal expansions, Debye-Waller factors temperature dependence of mechanical properties like elastic constants. A deep understanding of the phonon behavior, especially that of a new materials, is a necessary condition for future technological developments. Recently it has been shown that phonons can be quit reliable obtained directly from the *ab initio* calculations using standard *ab initio* codes and the Phonon code bases on the direct method. One can obtain sufficiently accurate phonon frequencies for insulator, semiconductors, metals, molecular crystals, including system containing the 3d elements, and crystals showing magnetic properties. Recently, even phonons for actinide crystals were treated satisfactory. The present *ab initio* codes allow to treat strong electron correlation systems, and these approaches seems to be sufficient to find phonon frequencies for them.

The phonon studies can be expanded to surfaces, interfaces, multilayers, crystals with defects and impurities, etc. These systems require larger computer memory and speed, but in principle do not cause too much problems. This field , therefore, opens a huge research area to understand the phonon modifications in the mentioned systems, and hence the changes in the temperature dependences of many properties. Exploration of these areas have started already, and it is desirable to exchange experiences and focus the studies on the most essential items. And that is one of the topic of the proposed Workshop.

Let us look a little bit closer at the computer tools used to find phonon frequencies. One way of treating phonons in crystalline systems is to use the Hellmann-Feynman forces calculated for specifically perturbed supercells. During the Workshop the numerical tools which allow to carry out *ab initio* phonon calculations for the above mentioned systems will be made familiar to the participants. The purpose of this workshop is to offer an introduction to the fundamentals of phonon calculations performed on the basis of the standard *ab initio* codes. Using the Phonon program phonon frequencies and related quantities can be computed. Bulk crystals, even complex ones, require less computational effort, while defected crystals, and lower dimensional systems, having less symmetry, need considerable computer power. Since these

calculations can be parallelized, the cluster facilities can be effectively used for this purpose. Moreover, the finite temperature calculations, carried out, for example, within the quasiharminic approximation, require to repeat many similar runs for slightly different parameter, like pressure. Thus, using the above numerical tools and computer cluster technique we are just facing the moment to handle effectively from first-principles the finite temperature properties of most crystalline systems.

## 7.**Preliminary workshop programme:**

- *Ab initio* calculations and direct method for phonon computations
- Derivations of bulk material properties described by phonons
- Phonons in hydrogen storage materials, actinides, and minerals
- Crystal defects and phonons
- Phonons on surfaces, decorated surfaces and interfaces
- Phonon-electron-magnetic interaction.

## 8.**List of participants:**

(not agreed tentative list of participants in alphabetic order)
(potential speakers are denoted by *)

- Adeagbo Waheed, University Duisburg-Essen, *
- Blaha Peter, Inst.Materials Chem. TU Vienne *
- Cerny Miroslaw, Brno Univ.Technology, Brno
- Chumakov Alexandre, ESRF, Grenoble
- Colakoglu Kemal, Gazi Univ. Ankara *
- Cottenier Steffan, Univ. Leuven, Leuven *
- De Boissieu Marc, CRNS, Grenoble *
- Delaire Olivier, Caltech, Pasadena *
- Fecher Gerhard, Johannes-Gutenberg Univ.
- Frankcombe Terry, Univ. Leiden, Leiden *
- Gregora Ivan, ASCR, Prague
- Hug Gilles LEM, ONERA-CNRS, Chatillon
- Johnson Mark, ILL, Grenoble *
- Kearley Gordon, Interfaculty Reactor Inst. Delf *
- Kresse Georg, Inst.Materialphysik, Univ.Vienne *
- Krisch Michael, ESRF, Grenoble *
- Kuwabara Akihide, Kyoto Univ. *
- Lovvik Martin, Univ.Oslo, Oslo *
- Nash Patrick, Univ. Texas, San Antonio *
- Shang Shunli, Pennsylvania State Univ. *
- Steinle-Neuwmann, Bayerisches Geoinstitut, Bayreuth *
- Stumpf Ronald, Meterials Physics, Sandia National Lab. *
- Schowalter Marco, Univ.Bremen, Bremen *
- Takamura Hiroshi *
- Teweldeberhan Amanuel, PTG, NMRC, Cork *
- Tse John, Univ.Saskatchewan, Saskatoon *
- Xuezhi Z.Ke, Univ. Nevada, Las Vegas *
- Wolf Walter, Materials Design Comp. *

9.**Estimated budget:**

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| - 4 Speakers hotel (3 nights: a 200 EU) - | 800,- EU |
| - 4 Speakers flights (flight: a 400 EU) - | 1200,- EU |
| - Computer rooms - | 200,- EU |
| - Bus (Institute <-> University**) - | 200,- EU |
| - Administration - | 300,- EU |
| TOTAL | 2700,- EU |

10.**Brief curriculum vitae of the principal applicant:**

Krzysztof PARLINSKI

- 1962, Grad. (mgr, M.Sc.), Physics, Jagiellonian University, Cracow.
- 1966, Ph.D Jagiellonian University, Cracow, Doctor Thesis "Dynamics of crystal lattice with librational degree of freedom".
- 1974, Dr Habilitation, Jagiellonian University, Cracow. "Application of the method of moments to description of liquid He4".
- 1975, Docent at Institute of Nuclear Physics, Cracow.
- 1986, Professor at the Institute of Nuclear Physics, Cracow.

***Long term stays***

- 1970, University of Edinburgh
- 1981, 1983, University of Antwerp, Incommensurate phases and phase transitions of molecular crystals.
- 1984, 1987 Laboratoire de Physique des Solides, l'Universite Paris-Sud, Orsay, Symmetry changes in incommensurate phases. Kinetics of incommensurate phases and quasicrystals.
- 1984, 1985, Kernforschungsanlage, Institut fur Feskorperforschung, Julich, Computer simulation and neutron scattering experiments on crystalline glasses and incommensurate phases.
- 1990, Institute Laue-Langevin, Grenoble, Neutron scattering on incommensurate crystals.
- 1994, 1997 Institute for Materials Research, Tohoku University, Kinetics of ferroelastic domain patterns. Lattice dynamics and relation to first-principle calculations.

***Scientific activities***

- Recent scientific activities: The main effort has been directed on studies of crystal structures, phase transitions, and lattice dynamics of crystals using the *ab initio* approach. Systems of general interests were studied: cubic ZrO2 ceramic-base material, hexagonal GaN used in light diodes, rhombohedral LiNbO3 applied in opto-electronic devices, tetragonal CuInSe2, AgGaSe2, AgGaTe2, CuInS2, CuFeS2,  ZnSnP2 used also in solar cells, tetragonal SnO2, GeO2 - a crystal similar to stishovite,

cubic TiC and ZrC - carbide crystals, cubic MgO, MgSiO3, Mg2SiO4, CaTiO3 - a geological important material, molecular crystals OC(NH2)2, hard material BN, other crystals ZnTe, FeBO3, beta-FeSi2, CaCl2, HgSe, Al2O3, NiTi shape memory alloy, intermetallics NiAl, TiAl, actinides UCoGa5, PuCoGa5, surfaces phonons on MgO(001), and in multilayers FeSI/Fe. For that crystals the phonon dispersion curves and phonon density of states has been calculated using the direct method.

- Written a software, called PHONON (http://wolf.ifj.edu.pl/phonon/), which incorporates the idea of the direct method, and allows to calculate phonon dispersion relation and phonon density of states for any crystal, surface via slab method, multilayers and defected systems which can be represented by a supercell. The calculated phonon dispersion curves agree quite well (within 5% in frequency) with the coherent inelastic neutron and x-ray scattering measurements, and Raman and infrared data. Software PHONON is used in a considerable number of Universities and Research Institutes all over the World. It was already used as a essential computational tool in about 100 publications.

- Maria Sklodowska-Curie Award in Physics of Polish Academy of Sciences, 2005. (considered as polish highest award for physicist)
- about 200 publications in International Journals.
- about 50 invited talks on International Conferences.
- about 70 seminars in foreign Universities and Research Institutes.
- promoting to PhD 3 students and 1 habilitation
- Referee for International Journals, PhD, habilitation thesis and promoting Professors
- Chairmen of 3 International Workshops
- Member of the International Union of Pure and Applied Physics,
- Head of the Department of Materials Research by Computers at the Institute of Nuclear Physics in Cracow,
- older scientific activities were in the fields of computer simulation, crystalline glasses, incommensurate phases, kinetics of phase transitions, theory of phase transitions, group theory, molecular crystals, quasicrystals, liquid helium, classical liquids, crystals with impurities, experimental neutron scattering on crystalline materials, high Tc superconductivity, domain structures of ferroelastics, direct method of lattice dynamics, calculation of lattice dynamics of crystals from first-principles. Analysis of phase transitions from first-principles.

**Five recent publications:**

1. P.Piekarz, K.Parlinski and A.M.Oles, The mechanism of the Vervey transition in magnetite, Phys.Rev.Lett. in print.
2. K.Parlinski, Structural phase transition in FeBO3 under pressure, Eur. Phys. J. B27, 283 (2002).
3. K.Parlinski and M.Parlinska-Wojtan, Lattice dynamics of NiTi austenite, martensite and R-phase, Phys. Rev. B66, 064307 (2002).
4. K.Parlinski, P.T.Jochym, O.Leupold, A.I.Chumakov, R.Ruffer, H.Schober, A.Jianu, J.Dutkiewicz, and W.Maziarz, Local modes of Fe

and Co atoms in NiAl intermetallics, Phys. Rev. B70, 224304-1-5 (2004).
5. M. Sternik, K. Parlinski, Lattice vibrations in cubic, tetragonal, and monoclinic phases of ZrO_2, J. Chem. Phys. 122, 064707-1-6 (2005).

11.**Acronym of the Standing Committee into whose domain your proposal:**

PESC

Krzysztof Parlinski Cracow, 29 September, 2006