

Proposal for a workshop funded by ESF Psi-k program

1. Title: Ab-initio approaches to electron-phonon coupling and superconductivity.

Abstract: The aim of this workshop is to give an overview of recent ab-initio calculations of electron-phonon coupling in superconducting and nonsuperconducting materials, in the bulk as well as at the surface. From methodological point of view the workshop will cover linear response calculations of the electron-phonon coupling resolved both in energy and momentum, the newly developed superconducting density functional theory, and numerical methods of the Eliashberg theory. Important topics like anharmonicity, nonadiabaticity, and unconventional order parameters will also be discussed, as well as spectroscopic effects of the electron-phonon coupling, e.g., in photoemission.

Organisers:

Prof. Dr. Ole K. Andersen
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2. Scientific summary:

The rich variety and complexity of superconducting materials and strong dependence of critical temperature and transport properties on electron and phonon structure of these materials requires ab-initio methods which treat electrons, phonons, and electron-phonon interaction on the same footing. The last decade was characterized by rapid progress in first principle calculations of electron-phonon coupling and related effects. This movement forward was achieved through advances in available computer power and invention of new theoretical methods, such as the theory of the order parameter density functional theory. Striking examples of this progress are the leading role played by theory in understanding the two-band superconductivity in MgB₂, and the unique superconductivity in doped diamond, rapid progress in understanding the novel intercalated superconductors based on first principle calculations, predictions related to superconductivity and lattice stability in hexagonal Li₂B₂, theory of superconductivity in compressed Li and Y. In the field of phonon-mediated superconductivity we have just made the leap that for the high-T_c cuprates still lies in the future: the field has moved from a "theory of superconductivity" to a "theory of superconductors", that is to say, a quantitative understanding of the principles controlling the superconducting properties of individual materials and developing a capability of predicting new superconductors.

The aim of the proposed workshop is twofold, first it should give an overview of the current status of the field, discuss the "hottest" novel electron-phonon superconductors, including (1) intercalated graphites and graphene-based borides, (2) newly discovered superconductors under ultrahigh pressure with record T_c among elemental metals, and (3) electron-phonon coupling effects in unconventional superconductors, such as ruthenates or non-centrosymmetric superconductors. In addition, electron-phonon coupling in low-dimensional geometries (thin films, interfaces, nanotubes, particles) will be an important focus of discussion. Due to a mix of invited speakers from theory and experiment, it will be clarified which information can be obtained from first-principles calculations and how this information can be experimentally tested and verified. Finally, since we have reached a new high level of computational capabilities, it seems appropriate to look forward and define future directions of research in this field. The proposed workshop in 2007 would be a very timely opportunity to fulfill that goal.

Second, young researchers participating in the workshop will be able to learn about the descriptive and predictive power of the modern ab initio methods, how and where they can be applied, what information can be obtained and where possible limitations will be. This should also help researchers to understand electronic structure calculations better and enable them to use these methods in future work.

3. Tentative list of speakers:

Name	Topic	Country
Akimitsu J.	Synthesis routes for possible new superconductors	Japan
Bachelet G.	CaAlSi and related materials	Italy
Boeri L.	CaC6: calculations of electron-phonon coupling and thermodynamics	Germany
Bohnen K.-P.	Lattice dynamics and electron-phonon coupling in carbon nanotubes	Germany
Calandra M.	Intercalated graphites under pressure	France
Christensen N.E.	Superconductivity in compressed alkali metals	Denmark
Curtarolo S.	Prediction of Li2B2, a stable superconducting analogue of MgB2	USA
Drechsler S.L.	Electron-phonon and electron-paramagnon coupling in MgCNi3	Germany
Eiguren A.	Electron-phonon interaction at the metal surfaces: theory	Spain
Goldoni A.	Spectroscopy of fullerenes and nanotubes	Italy
Golubov A.A.	Applications of anisotropic Eliashberg theory	Holland
Gonnelli R.	Point-contact spectroscopy of e-p coupling in MgB2	Italy
Gross E.K.U.	Superconducting density functional theory	Germany
Hofmann Ph.	Electron-phonon interaction at metal surfaces: experiment	Denmark
Johannes M.D.	Electron-phonon coupling and charge density wave instabilities	USA
Karpinski J.	Effect of Al-Li co-doping on e-p coupling in MgB2	Switzerland
Kortus J.	Recent advances in the first-principles calculations for MgB2	Germany
Kremer R.	Specific heat and coherence length in CaC6: implications for the electron-phonon coupling	Germany
Littlewood P.B.	Superconductivity in intercalated graphites	UK
Liu A.Y.	Electron-phonon coupling in Li2B2	USA
Louie S.G.	Phonons in carbon nanotubes	USA
Massida S. A.	Impurity effects in superconductivity of MgB2	Italy
Mauri F.	Anharmonic effects in superconductivity	France
Saxena S.S.	Experimental aspects of superconductivity in intercalated graphites	UK
Sklyadneva I.Yu.	Ab-initio calculations of electron-phonon coupling at metal surfaces	Spain
van der Marel D.	Electron-phonon effects in optics of MgB2	Switzerland

4. Number of participants:

- ~25 invited speakers with a mix of theory and related experiment
- 35 young scientists

total 60 participants

5. Tutorial element

There are several codes available for electronic structure calculations together with linear response method in order to calculate the electron-phonon interaction from first-principles. Other codes based on recently proposed superconducting density functional theory (SDFT) have been recently developed. An important component of the toolbox of the modern band theorist working with superconductors are codes for the solving of anisotropic, multiband Eliashberg equations. We anticipate having tutorials on using the PW-SCF (“quantum espresso”) code for linear response and/or for SDFT calculations. Tutorial day will be either immediately after or immediately before the workshop.

6. Budget

There will be no registration fee in order to attract younger researcher.

The living expenses and depending on funding also part of the travel costs of the invited speakers will be covered.

Hotel: 3 nights*25 speakers * 100 EUR = 7500 EUR

Travel: 15000 EUR

Social dinner: 2000 EUR

Misc.: 500 EUR

estimated Total cost 25000 EUR

We would like to ask ESF Psi-k to cover 10000 Euro.

7. Statement of co-sponsorship of other organizations and additional funding.

Donostia International Physics Center (DIPC) and the University of the Basque Country will provide funding of 10000 Euro. DIPC will also provide the meeting room and local organization.

We are applying for support from NSF International Materials Science program (5000 Euros).

8. Place of workshop

Donostia International Physics Center (DIPC),
San Sebastian/Donostia, Basque Country, Spain
DATE: 28 May 2007 - 30 May 2007

9. Support for American participants

Some American participants will be supported by the co-sponsorship of DIPC and NSF.

Ole K. Andersen.

Education

1966 Masters Degree in Electronic Engineering, Technical University of Denmark, Department of Electrophysics

1969 Technical Licentiate in Solid State Physics; Technical University of Denmark, Department of Electrophysics.

Professional Employment

1969-70 Research Associate; University of Pennsylvania, Physics Department.

1970-72 Universitetsadjunkt (~ Assistant Professor); University of Copenhagen, Orsted Laboratory, Department of Solid State Physics.

1972-78 Lektor (~ Associate Professor); Technical University of Denmark, Department of Electrophysics.

1978- Director at the Max-Planck-Institut für Festkörperforschung in Stuttgart Managing Director 1983-85, 1997-99.

Honors and Memberships

1978 Brinch Prize; Danish Physical Society.

1980 Hewlett-Packard Europhysics Prize; European Physical Society.

1978 Scientific Member of the Max-Planck-Society.

1982 Honorary Professor; University of Stuttgart, Physics Faculty.

1982 Foreign Member of the Royal Danish Academy of Sciences.

1992 Foreign Member of the Ukrainian Academy of Sciences.

1993 Fellow of the American Physical Society.

Publications statistics

180 publications, of them 24 in Puz. Rev. Let., Nature or Science.

Approximately 15700 citations; Hirsch index 57

Five recent publications most closely related to this proposal

1. [Three-dimensional MgB₂-type superconductivity in hole-doped diamond](#), L. Boeri, J. Kortus, O.K. Andersen, Phys. Rev. Lett. **93**, 237002 (2004)
2. First-principles calculation of the superconducting transition in MgB₂ within the anisotropic Eliashberg formalism, I. Mazin, O.K. Andersen, O. Jepsen, Golubov AA, Dolgov OV, Kortus J, Phys. Rev **B69**, 056501 (2004)
3. Pressure dependence of electron-phonon coupling and superconductivity in hcp Fe: A linear response study, S. K. Bose, O. V. Dolgov, J. Kortus, O. Jepsen, and O. K. Andersen Phys. Rev. B **67**, 214518 (2003)
4. Superconductivity in MgB₂: Clean or Dirty? I. I. Mazin, O. K. Andersen, O. Jepsen, O. V. Dolgov, J. Kortus, A.A. Golubov, A.B. Kuzmenko, D. van der Marel, Phys. Rev. Lett. **89**, 107002 (2002)

5. Specific heat of MgB₂ in a one- and a two-band model from first-principles calculations, A A Golubov, J Kortus, O V Dolgov, O Jepsen, Y Kong, O K Andersen, B J Gibson, K Ahn and R K Kremer, *J. Phys.: Condens. Matter* 14, 1353 (2002)

Evgueni V.Chulkov

Education

M.Sc., 1974, Tomsk State University, Tomsk, USSR

Ph.D., 1980, Tomsk State University, Tomsk, USSR

Professional Employment

1974-84, Junior researcher, Siberian Institute of Physics and Technology, (Tomsk).

1979-84, Researcher, Institute of Atmospheric Optics, USSR Academy of Sciences, (Tomsk).

1984-88, Senior Researcher, Institute of Strength Physics and Materials Science, USSR Academy of Sciences, (Tomsk).

1988-95, Director of Laboratory for Physics of Surface Phenomena, Institute of Strength Physics and Materials Science, USSR Academy of Sciences, (Tomsk).

1995-96 Sabbatical, Spanish Ministry of Education and Culture, University of the Basque Country, Chemical Faculty, Materials Physics Department, San Sebastián, Spain.

1996-2000 Visiting Professor of the Basque Country Government, University of the Basque Country, Chemical Faculty, Materials Physics Department, San Sebastian, Spain.

2000- Professor of the University of the Basque Country, Chemical Faculty, Materials Physics Department, San Sebastian, Spain.

Publication Statistics

200 publications, of them 15 in Phys. Rev. Lett. and Science.

Approximately 2000 citations; Hirsch index 22

Five recent publications most closely related to this proposal

1. Electron-phonon contribution to the phonon and excited electron (hole) linewidths in bulk Pd, I.Yu.Sklyadneva, A.Leonardo, P.M.Echenique, S.V.Eremeev, and E.V.Chulkov, *J. Phys.: Condens. Matter*, **18**, 7923 (2006).
2. The electron-phonon coupling on Mg(0001), T.K.Kim, T.S.Sørensen, E.Wolfring, H.Li, E.V.Chulkov and Ph.Hofmann, *Phys. Rev. B*, **72**, 075422 (2005).
3. Electron-phonon interaction at the Be(0001) surface, A.Eiguren, S. de Gironcoli, E.V.Chulkov, P.M.Echenique, and E. Tosatti, *Phys. Rev. Lett.*, **91**, 166803 (2003).
4. Electron-phonon coupling at metal surfaces, B.Hellsing A.Eiguren, and E.V.Chulkov, *J.Phys.Cond.Matter*, **14**, 5959 (2002), (Review).

5. Role of bulk and surface phonons in the decay of metal surface states, A.Eiguren, B.Hellsing, F.Reinert, G.N.Nicolay, E.V.Chulkov, V.M.Silkin, S.Hüfner, and P.M.Echenique, Phys. Rev. Lett, **88**, 066805 (2002).

Igor I. Mazin

Education

M. Sc., Metal Physics, 1977, Moscow Institute for Steel and Alloys, Moscow, USSR
Ph.D., Theoretical Physics, 1984, P.N. Lebedev Physical Institute, Moscow, USSR

Professional Employment

77-84 Engineer, Institute of Metallurgy, Moscow, USSR
84-91 Junior Researcher, Researcher, P.N. Lebedev Physical Institute, Moscow, USSR
91-94 Staff Member, Max-Planck Institute for Solid State Research, Stuttgart, Germany
94-96 Senior Research Associate, Carnegie Institution of Washington, Washington,

96-98 Research Professor, George Mason University, Fairfax, Virginia D.C.
98- Research Physicist, Naval Research Laboratory, Washington, D.C.

Honors and Memberships

USSR State Prize for Young Scientists (1989)
A. von Humboldt Fellowship (1989)
Center for High Pressure Research Fellowship (1994)
Alan Berman NRL best publication award (1997, 2006)
2005 Fellow of the American Physical Society.

Publications statistics

160 publications, of them 26 in *Phys. Rev. Lett.*, *Nature* or *Science*.
Approximately 4500 citations; Hirsch index 35

Five recent publications most closely related to this proposal

1. Phase-sensitive tests of the pairing state symmetry in Sr_2RuO_4 , Igor Zutic and Igor Mazin, *Phys. Rev. Lett.* **95**, 217004 (2005).
2. Intercalate driven superconductivity in CaC_6 and YbC_6 , I. I. Mazin, *Phys. Rev. Lett.* **95**, 227001 (2005).
3. Critical temperature and giant isotope effect in presence of paramagnons, O.V. Dolgov, I.I. Mazin, A.A. Golubov, S.Y. Savrasov, and E.G. Maksimov, *Phys. Rev. Lett.* **95**, 257003 (2005).
4. Electronic Structure and Electron-Phonon Coupling in the 18K Superconductor Y_2C_3 , D.J. Singh and I. I. Mazin, *Phys. Rev.* **B70**, 052504 (2004)
5. Electronic structure and superconductivity of CaAlSi and SrAlSi , I.I. Mazin and D.A. Papaconstantopoulos, *Phys. Rev.* **B69**, 180512 (2004).

Warren E. Pickett

Education

PhD 1975 SUNY Stony Brook
MS 1971 Wichita State University
BS 1969 Wichita State University

Professional Employment

75-76 Postdoctoral appointment, University of Bristol, England
76-77 Postdoctoral appointment, UC Berkeley
78-79 Postdoctoral appointment, Northwestern University
79-97 Research scientist, Naval Research Laboratory, Washington, D.C.
97- Professor, UC Davis

Honors and Memberships

Sigma Xi Technical Achievement Award in Pure Science, 1993
Alan Berman NRL Research Publications Award, 1983, 1988, 1989, 1992
E.O. Hulbert Award, Naval Research Laboratory, 1990
Second Prize in IBM Supercomputing Competition - Mathematics and Physics, 1990
Named to Top Ten Technology Talents of 1989 Washington Technology
Elected Fellow of the American Physical Society, 1989
Scientific Achievement Award, Washington Academy of Sciences, 1985
1989: Fellow of the American Physical Society

Publications statistics

Over 350 publications, of them 55 in Phys. Rev. Lett., Nature or Science.
Approximately 9500 citations; Hirsch index 48

Five recent publications most closely related to this proposal

1. Superconductivity and Lattice Instability in Compressed Lithium from Fermi Surface Hot Spots, D. Kasinathan, J. Kunes, A. Lazicki, H. Rosner, C. S. Yoo, R. T. Scalettar, and W. E. Pickett. Phys. Rev. Lett. 96, 047004 (2006)
2. KOs₂O₆: Superconducting rattler, J. Kunes, W.E. Pickett, Physica B, **378-80**, 898-899 (2006).
3. Crystal symmetry, electron-phonon coupling, and superconducting tendencies in Li₂Pd₃B and Li₂Pt₃B, K.-W. Lee and W. E. Pickett, Phys. Rev. B 72, 174505 (2005)
4. Superconductivity in boron-doped diamond, K.-W. Lee and W. E. Pickett. Phys. Rev. Lett. 93, 237003 (2004).
5. Prediction of High T_c Superconductivity in Hole-Doped LiBC, H. Rosner, A. Kitaigorodsky, and W. E. Pickett. Phys. Rev. Lett. 88, 127001 (2002)