SUMMARY

Workshop "*Ab-initio* approach to electron-phonon coupling and superconductivity" was held at Donostia International Physics Center, San Sebastian, the Basque Country, Spain, 28/05/2007 – 30/05/2007 .

Organizing Committee, which consisted of Prof. O.K.Andersen, Prof. E.V.Chulkov, Dr.I.I.Mazin, Prof.W.E.Pickett, and A.Leonardo, invited 23 theoretical and experimental experts to give an overview of:

1) recent ab-initio calculations of electron-phonon coupling in bulk superconducting and not superconducting materials as well as at surfaces of these materials;
2) effects of electron-phonon coupling in photoemission and other techniques measurements;
3) various chemical aspects that influence the superconductor materials growth.

Total number of presentations was 36 (23 oral presentations – invited speakers and 13 poster presentations). Total number of participants was 43 from nine European Countries (Denmark, England, France, Germany, Italy, Russia, Spain, Sweden, and Switzerland) and from US.

Oral presentations were distributed over 9 sessions and covered large variety of materials ranging from LiB and graphene to very complex intercalated zirconium and hafnium nitride halides potentially interesting for superconductivity. Of particular interest were presentations of theoretical and experimental studies of electron-phonon interaction on metal surfaces since electron-phonon coupling on surfaces can be very distinct on that in bulk materials. Poster presentations covered such interesting problems as a role of phonon softening and anharmonicity in the lattice instability and electron-phonon coupling in complex materials as well as electron-phonon interaction in metal adlayers and in bulk metals under high pressure.

The meeting provided a nice atmosphere for fruitful discussions and an initiation of collaborations between different groups.

Highlights of the meeting

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. Rapid progress in first principle calculations of electron-phonon coupling and related effects has been achieved during the last decade. The present workshop is aimed to give an overview of the current status of the field, discuss the "hottest" novel electron-phonon superconductors, including (1) intercalated graphites, (2) newly discovered superconductors under ultrahigh pressure with record Tc among elemental metals, and (3) electron- phonon coupling effects in unconventional superconductors, such as alkali osmates. In addition, electron-phonon coupling in low-dimensional geometries (thin films, interfaces, nanotubes, particles) is an important focus of discussion. Due to a mix of invited speakers from theory and experiment, it is clarified which information can be obtained from first-principles calculations and how this information can be experimentally tested and verified.

Day 1

In the first talk of the workshop K.-P. Bohnen discussed lattice dynamics and electron-phonon interaction in small diameter carbon nanotubes. He showed that all ab-initio calculations for *isolated* nanotubes with diameter of 4 Å demonstrate a strong tendency to either a Peierls transition or a structural transition to a non-metallic state with a small gap, in contrast to experimental findings. Even with doping these calculations favour the Peirels transition compared to superconductivity. The conclusion of the talk is that other physical aspects like interaction with the zeolite crystal, possible defects etc. should be considered to describe the experimentally found superconductivity transition.

A number of impressive talks has been devoted to the study of electron-phonon (e-ph) interaction and superconductivity in graphite intercalated systems (GIS). G. B. Bachelet, M. Calandra, and L. Boeri addressed theoretical aspects of superconductivity in CaC_6, YbC_6, SrC_6, MgC_6, and BaC_6, wheares J. S. Kim and M. Ellerby discussed experimental studies of these compounds. G. B. Bachelet presented a simple model that captures essential features of the e-ph properties of GISs and explains the empirical correlation between the filling of the interlayer band and the occurance of superconductivity in GISs. Calandra and Boeri discussed superconductivity in GISs by using ab-initio calculation results for electron band structure and e-ph coupling.
In particular, it was shown, that CaC6 should be superconducting with Tc =11 K while for Ba and Sr intercalated graphite Tc was found to be 0.2 K and 3.0 K, respectively. The latter values were recently confirmed experimentally. Experimental measurements, reviewed by Kim and Ellerby, confirmed the idea of an anisotropic superconducting gap in alkaline-earth GISs and e-ph mechanism of superconductivity in these systems.

R. S. Gonnelli and S. Massida in their interesting talks discussed impurity effects on superconductivity in MgB_2. They showed both theoretically and experimentally that impurities and disorder lead to a strong decrease in the –band e-ph coupling. F. Mauri and A. Goldoni discussed intriguing questions of non-adiabatic vibrations in doped graphene and angle-resolved photoemission measurements of electronic structure of $K_6C_{60}(110)$ and $K_3C_{60}(111)$ films.

D. A. Papaconstantopoulos and A. Bergara presented fascinating discussion of superconductivity in bulk metals under pressure. In particular, Papaconstantopoulos by using band theory, McMillan approach, and the rigid-muffintin theory performed systematic study of superconducting properties in many metals and showed the systemic increase of critical temperature and e-ph coupling with pressure. Bergara discussed superconductivity in alkali metals. Basing on ab-initio calculations he showed that under pressure in alkali metals a soft phonon mode arises in FCC alkalis along ΓK direction. This softening increases e-ph coupling under pressure and, respectively, increases critical temperature Tc.

Day 2

This day sessions have been devoted to three topics: many-body effects in superconductivity, e-ph interaction on metal surfaces and in adlayers, and superconductivity in lithium boride compounds. E.K.U. Gross presented impressive review of the recently developed density-functional-type method for the description of phonon-mediated superconductivity. This method treats e-ph interaction and electron-electron repulsion on the same footing thus avoiding any adjustable parameters. Gross also reviewed recently obtained numerical results for critical temperature in simple metals and MgB2, including Li, K, and Al under pressure. He explained why Li and Al behave very differently under pressure: in bulk Li pressure leads to a strong enhancement of superconductivity while in Al pressure suppresses electron-phonon coupling. A remarkable result of the new theory is a two-gap superconductivity in Pb somewhat similar to MgB_2.

In the very interesting talk of O.Gunnarsson the e-ph interaction have been discussed for strongly correlated systems. An important point of the discussion was whether correlation enhances or suppresses the e-ph coupling. It is normally assumed on one hand that correlation suppresses the e-ph coupling. On the other hand it is argued that antiferromagnetic correlation enhances the e-ph interaction. These issues were discussed and it was argued that the effect of the e-ph interaction depends crucially on which phonons are considered and which property is studied.

D. Van Der Marel reviewed recent comprehensive experimental study of a relatively simple perovskite compound $SrTi_{1-X}Nb_XO3$ for small X. The goal of this study was to what extent electron-phonon coupling is important for the transport anomalies and superconductivity in perovskites. The analysis of the obtained results for $SrTi_{1-X}Nb_XO3$ showed that the e-ph coupling parameter is of intermediate strength. This

assumes that the electron-phonon coupling does not play major role in superconductivity of perovskites.

The session devoted to the e-ph interaction on metal surfaces started with the talk by Ph.Hofmann. In the very informative style he reviewed angle-resolved photoemission measurements of e-ph coupling in surface states on metal surfaces performed during the last decade. He outlined advantages and disadvantages of photoemission technique in the study of e-ph interaction on metal surfaces. In particular, he emphasized the possible role of thermal defects which can make difficult the accurate interpretation of e-ph interaction. He sowed that on many surfaces the e-ph coupling is much stronger than in bulk metal.

A.Eiguren discussed his ab-initio calculation results for a hydrogen covered W(110) surface. B.Hellsing discussed the calculations of phonon induced lifetime widths of photo holes and e-h pair excitation driven liftetime broadening as well as the shift of particular phonon modes. He also reviewed recent DFPT phonon calculations of Cu(111) and Cs/Cu(111) and the importance of e-p coupling for hydrogen vibrational modes of the system H/W(110). I.Yu.Sklydneva presented the ab-initio calculation results for electron-phonon coupling in the Γ and X surface states on the Al(001) surface and the contribution of e-ph scattering to the hole (electron) lifetimes in these states. The Al(001) surface can be be considered as a reference one since both electron and phonon structures of the surface are well known both experimentally and theoretically. Additionally, very recently the e-ph copling parameter has been measured for the Γ surface state. Sklyadneva showed that e-ph coupling is is very distinct in the considered surface states. However, in both states the coupling shows only weak momentum and energy dependence.

S. Curtarolo discussed in his presentation theoretical study of thermodynamic stability and electronic properties of layered metal borides, leading to the prediction of a hypothetical novel superconductor Metal Sandwich – LiB. It was demonstrated that the peculiarities of MS-LiB in terms of electronic structure, layer arrangements and doping capabilities allow a lot of freedom in the search for higher T_c systems.

A.Y. Liu presented recent theoretical results obtained in collaboration with I.I.Mazin for e-ph coupling in a hypothetical layered lithium monoboride, Li_2B_2. She showed that despite this material combines features of both MgB_2 and CaC_6 the e-ph coupling in Li_2B_2 is weaker than in MgB_2. This effect is related to the lack of π electron states at the Fermi level. She argues that these states can be restored at the Fermi level through doping or pressure.

Poster presentations of the workshop can be separated into few groups:
1) presentations, where the critical temperature Tc is the main point of the study;
2) presentations where e-ph coupling is used for analysis of related phenomena;
3) presentations where phonons play important role in different properties, for instance in lattice instabilities;

4) the rest.

W.E. Pickett discussed in his presentation the critical temperature Tc behaviour under pressure in yttrium and calcium. He showed that e-ph coupling strength increases substantially under pressure in yttrium. He concludes from linear response calculations that simple cubic Ca is strongly unstable in the entire pressure range of interest.

S.V. Eremeev discussed the e-ph coupling in a quantum-well state formed by one monolayer of sodium on Cu(111) and the e-ph scattering contribution to the hole lifetime. M.D. Johannes presented the analysis of the role of the e-ph coupling in charge density wav transitions while R.S. Sanchez-Carrera discussed the e-ph interaction in organic semiconductors and the effect of this interaction on charge transport.

A. Ayuela discussed the phonon softening effect on instabilities in magnetic-shape-memory alloy Ni_2MnGa. M.Calandra analysed the role of anharmonicity and non-adiabatic effects in MgB_2. R.Heid presented the discussion of the observed anomalous phonon properties of the oxygen stretching modes and the relation to the e-ph coupling in the YBCO family materials. M.Lüders presented the ab-initio description of the isotope exponent.

F.Binder discussed the role of magnetism in the structure formation of transition-metal nanosystems. I.I.Mazin discussed charge ordering effect as alternative to Jang-Teller distortion in the rare earth nickelates. S.V.Streltsov studied nonadiabatic renormalization effects in optical phonon frequencies and lineshape in osmium by measuring the electronic Raman response of osmium at pressure up to 60 GPa. M.G.Vergniory presented an analysis of the electronic resonse on magnesium surface.

Day 3

O. Fischer reviewed recent scanning tunnelling spectroscopy stydies of a number of materials from the Chevrel phases family. In particular, from measuring the quasiparticle DOS it is concluded that the temperature dependence of the gap is incompatible with a conventional isotropic s-wave interpretation.

J. Kunes presented an overview of the current knowledge on alkali osmates and focused on the peculiar lattice dynamics in potassium osmate, its theoretical description and possible consequences.

A. Fuertes presented an interesting overview of chemistry and crystal structure of superconducting layered zirconium and hafnium nitride halides. She discussed different aspects of the intercalation chemistry in these systems focussing on the relation ships between the chemical composition of the hosts, their defect structure, the staging phenomenon, and superconducting properties of the intercalates.

Assessment of the results …

The workshop presentations and the respective discussions have shown rapid progress in understanding of superconductivity based on theoretical (ab-initio) and experimental study of electron-phonon (e-ph) interaction. This progress is related to the study of novel electron-phonon superconductors, including (1) intercalated graphites and graphene-based borides, (2) newly discovered superconductors under ultrahigh pressure with record Tc among elemental metals, and (3) electron- phonon coupling effects in unconventional superconductors, such as ruthenates or non-centrosymmetric superconductors.
Another important aspect of the e-ph coupling rapidly developed last years is the role of this coupling in the excited electron and hole lifetimes in bulk metals and at metal surfaces. It was shown that the e-ph coupling contribution to the electron lifetime broadening is very often comparable to the electron-electron inelastic contribution and at room temperature can be even dominant.

Important conclusions of the workshop:

1. In addition to the e-ph coupling in small diameter carbon nanotubes other physical aspects like interaction with the zeolite crystal, possible defects etc. should be considered to describe the experimentally found superconductivity transition in the nanotubes.

2. Alkaline-earth graphite intercalated compounds exhibit an anisotropic energy gap and pairing mechanism in these compounds is due to e-ph interaction.

3. Both theory and experiment demonstrate that impurities and disorder lead to a strong decrease in the –band e-ph coupling of MgB_2.

4. Adiabatic approximation fails to describe phonon properties of graphene.

5. Ab-initio calculations show that under pressure in alkali metals a soft phonon mode arises in FCC alkalis along ΓK direction. This softening increases e-ph coupling under pressure and, respectively, increases critical temperature Tc.

6. A two-gap superconductivity in Pb somewhat similar to MgB_2 is obtained from density functional calculations.

7. Experimental study of simple perovskite compounds demonstrates that the electron-phonon coupling does not play major role in superconductivity of perovskites.

8. Both experimental and theoretical studies show that the electron-phonon coupling on many metal surface is much stronger than in bulk metals.

9. Scanning tunnelling spectroscopy studies of a number of materials from the Chevrel phases family show that the temperature dependence of the gap is incompatible with a conventional isotropic s-wave interpretation.

Future developments

1. Study of other (than e-ph coupling) mechanisms of superconductivity in carbon nanotubes.

2. Investigations of non-adiabatic effects in vibrations of doped grapheme.

3. Applications of density functional theory to the study of superconductivity in high Tc materials.

4. Further search of new superconducting materials.

PROGRAM

Ab-initio approaches to electron-phonon coupling and superconductivity

San Sebastian – Donostia, May 28-30, 2007

Monday, May 28, 2007

8:45 – 9:00 **Opening**

9:00 – 9:45 **K. P. Bohnen**
Lattice dynamics and electron-phonon coupling in carbon nanotubes

9:45 – 10:30 **F. Mauri**
Non-adiabatic vibrations in doped graphene

10:30 – 11:00 **A. Goldoni**
Band dispersion K_6 C_{60}(110) and K_3 C_{60}(111) films measured with angle-resolved photoemission

11:00 – 11:30 **Coffee Break**

11:30 – 12:00 **R. S. Gonnelli**
Point-contact Andreev-reflection spectroscopy and electron-phonon coupling in doped and irradiated MgB_2

12:00 – 12:30 **S. Massida**
Impurity effects in superconductivity of MgB_2

12:30 – 13:00 **G. B. Bachelet**
Electron-phonon interaction in electron-doped graphite

13:00 – 14:30 **Lunch**

14:30 – 15:00 **M. Calandra**
Superconductivity in graphite intercalated with alkaline earths

15:00 – 15:30 **J. S. Kim**
Superconductivity in alkaline earth-intercalated graphites: CaC_6 and SrC_6

15:30 – 16:00 **L. Boeri**
Electron-phonon interaction in hexagonal layered compounds: alkali-earth intercalated graphites and disilicides

16:00 – 16:30 **M. Ellerby**
Experimental aspects of superconductivity in intercalated graphites

16:30 – 17:00 **Coffee Break**

17:00 – 17:30 **D. A. Papaconstantopoulos**
Effects of pressure on superconductivity in monoatomic metals

17:30 – 18:00 **A. Bergara**
Increasing crystal local-field effects and superconductivity in simple elements under pressure

Tuesday, May 29, 2007

9:00 – 9:45 **E. K. U. Gross**
How to predict the critical temperature of superconductors?

9:45 – 10:30 **O. Gunnarsson**
Many-body effects in electron-phonon coupling

10:30 – 11:00 **D. Van der Marel**
Electron-phonon interaction and charge carrier mass enhancement in n-doped $SrTiO_3$

11:00 – 11:30 **Coffee Break**

11:30 – 12:15 **Ph. Hofmann**
The electron-phonon interaction probed by angle resolved photoemission

12:15 – 12:45 **A. Eiguren**
Complex quasi-particle structure induced by electron-phonon interaction

12:45 – 14:30 **Lunch**

14:30 – 15:00 **B. Hellsing**
First principles surface phonons and electron and phonon lifetimes at surfaces

15:00 – 15:30 **I. Sklyadneva**
Ab-initio calculation of electron-phonon coupling at metal surfaces Al(001)

15:30 – 16:00 **S. Curtarolo**
First principle search for new superconducting materials

16:00 – 16:30 **A. Liu**
Electron-phonon coupling in Li_2B_2

16:30 – **Coffee Break and Poster Session**

20:30 - **Conference dinner**

Wednesday, May 30, 2007

9:00 – 9:45 **O. Fischer**
Scanning tunneling spectroscopy of Chevrel phases

9:45 – 10:30 **J. Kunes**
$K_6Os_2O_6$: superconducting rattler

10:30 – 11:00 **A. Fuertes**
Superconductivity in layered zirconium and hafnium nitride halides

11:00 – 11:15 **Closing**