Research Networking Programmes

Science Meeting – Scientific Report

The scientific report (WORD or PDF file - maximum of seven A4 pages) should be submitted online within two months of the event. It will be published on the ESF website.

Proposal Title: *(Towards) Room Temperature Superconductivity*

Application Reference N°: 5220

1) Summary

Obtaining a room-temperature superconductor has been one of the biggest challenges in solid state physics in the last hundred years. Achieving this goal would have enormous technological and economic implications, possibly leading to a new "industrial revolution". Decades of research have permitted to understand many peculiar properties of superconductors, leading to six Nobel prizes. However, despite the many efforts of theoretical physicists, all the discoveries of new classes of superconducting materials have happened by chance. The most recent example, after the cuprates, is that of Fe pnictides and chalcogenides, discovered accidentally in 2008. These are, to date, the two classes of compounds which reach the highest critical temperatures (T_c) – 160 and 60 K respectively. In these compounds, as well as in some other superconductors with lower T_c's, there is currently little consensus on fundamental issues, such as the very nature of the pairing mechanism. This strongly limits the predictive power of superconducting theories. On the other hand, the availability of an universally agreed on, unified theory, would open the way to real *ab-initio* theoretical predictions of high-temperature superconductors.

In the last few years, development of computing capabilities and methods for big data analysis have led to the development of *high-throughput* methods for material development. In these methods, large databases of *ab-initio* data are analysed to identify and optimize descriptors which correlate with a given physical properties. Combining high-throughput search with a predictive *ab-initio* theory of superconductivity is a strong shift of paradigm in the field, which could lead to an effective strategy for the search of better superconductors.

This was the main goal our workshop, which has brought together top researchers from different parts of the world and complementary expertises in the following fields:

- *Ab-initio* calculations for superconductors.

- Material synthesis (experimental) and prediction via *high-throughput* methods;

- Experimental characterization of the order parameter;

- Model Hamiltonians and many-body methods.

2) Description of the scientific content of and discussions at the event

Although several conferences and workshops took place in the last years having superconductivity as the main topic, most of them focused on the characterization of existing materials (recently, a strong focus has been given to the iron-based superconductors), or to specific models or scenarios for superconductivity. In fact, several communities exist in the field, which often employ competing views and methods, and it is rare that places or meetings exist where these views are confronted and challenged in an open atmosphere.

Our workshop had the concrete goal of designing a strategy to search for high-temperature superconductivity, starting from the experience gained in many years of research on actual materials. For this, we thought it would be important to bridge the gap between different communities and methods (*ab-initio* calculations, model Hamiltonians, experiments, material synthesis), and to include also experts of *high-throughput* methods, and new synthesis and techniques for the artificial design of new materials (field effect and polymer doping).

One of the main topic of discussion was the role of theoretical methods in this search, and the possibility of merging or combining the various model and *ab-initio* approaches to superconductivity to make them sufficiently predictive to form a solid basis for *high-throughput* simulations. Another very debated topic was how to condense the existing empirical knowledge in the field into a compact set of *descriptors*, to be exploited with *high-throughput* methods. While *high-throughput* experts demanded descriptors which are as simple and general as possible, experts in superconductivity have pointed out that most likely conventional (electron-phonon) and exotic (spin-fluctuations) superconductors would need different descriptors.

Furthermore, due to the presence of several experts, there was also a strong discussion on how to exploit new experimental techniques which permit to control structure and doping much more efficiently than traditional chemistry methods to optimize the superconducting properties of known materials. In particular, polymer gating, interfacing and heterostructures were discussed.

With this in mind the workshop has been structured in order to maximize open discussions on these topics. In order to estabilish a common ground for discussion for the different communities, representative experts have been asked to present detailed reviews on their fields. During the week of the workshop, there were five review talks on:

- Fundamentals of Superconductivity (*D.J. Scalapino*)

- Key Experiments (*P. Canfield*)
- Ab-initio Methods for Superconductors (*M. Cohen*)
- Model Approaches to Unconventional Superconductivity (Weak Coupling) (*P. Hirschfeld*)
- Unconventional (Topological) Superconductivity (*W. Hanke*)
- High-Throughput Methods (*S. Curtarolo*)

These review talks were allotted two hours, and participants were encouraged to interrupt the speakers with questions and comments. This proved to be a very effective format to stimulate the discussion. Besides the long review talks, each participant was offered to present his/her own results in a shorter (half an hour) talk; also in this case other participants were encouraged to interrupt the speakers with questions and comments. The program also included a few discussions on selected scientific papers or topics (journal club), and a round table in which we addressed provocative questions on superconductivity, ranging from fundamental questions to actual applications of room-temperature superconductors.

To summarize the discussion, the following general questions have emerged:

- How reliable are ab-initio calculations for superconductors?
- How easy is it to predict new conventional (electron-phonon) superconductors? What are the important material-specific properties? What is the role of thermodynamics?
- How far are we from a predictive power for spin-fluctuation mediated superconductivity? What is the problem in this case?
- What have we learnt about spin-fluctuations mediated superconductivity from the case of Fe superconductors?
- What is the role of other collective phenomena in exotic superconductors (nematic fluctuations, spin-orbit coupling etc)?
- How relevant are other superconducting mechanisms? Have they ever been observed?

On top of these questions, there has been a lot of discussion in the workshop on strategies to make the enormous existing knowledge systematic, in order to make it available for *high-throughput* analysis. This applies to both first-principle calculations and experimental data. Compiling and searching a database of this information, and identifying good possible descriptors, would also be extremely useful for future research. A few questions which have emerged in this sense are:

- What would be empirical good descriptors for conventional (i.e. phonon-mediated) superconductors? In this case, the present knowledge is so good that, in a few years, thanks to faster computer and implementation of electron-phonon calculations with Wannier functions, even full calculations of the critical temperatures could be used for high-throughput methods.
- What would be good descriptors for spin-fluctuation-mediated superconductivity? Is it actually necessary to have a quantitative theory for spin fluctuations to derive good descriptors, or would it be sufficient to use physical intuition?
- Empirical observation shows that superconductivity often occurs close to an instability in the phase diagram. This suggests that good “fishing spots” for superconductors are materials with incipient structural instabilities or fragile magnetism. Is it possible to find a way to quantify/characterize this empirical observation?

- Several low-T_c superconductors are presently known. Most likely, not all of these are phonon-mediated, but not all compounds are completely characterized. Identifying unconventional superconductors with low-critical temperatures might be a good way to pin-point interesting material classes, where superconducting critical temperatures could then be tuned by doping, strain, etc. This route is suggested by the recent case of Fe-based superconductors, where the observation of superconductivity with 7 K in LaFePO passed almost unobserved. Only two years later, with the report of a Tc of 28 K in LaFeAsO, the iron-age of superconductivity actually started, leading to the discovery of more than 100 new compounds with Tc's up to 60 K.

The construction such databases is a very ambitious project which would require a common effort of several researchers in the US and Europe. Part of the workshop has been used to suggest and discuss possible ways to increase cooperation in the field.

3) Assessment of the results and impact of the event on the future directions of the field

The workshop has been quite successful, in particular because the format was designed to encourage a collaborative and open atmosphere between all participants. The balanced mix between young and experienced researchers has further ensured that both traditional and model approaches to the field have been represented.
The interaction with the field of *high-throughput* methods has provoked an interesting "shift of paradigm" in the field, moving the focus from the discussion of possible models for pairing mechanism to actual physical systems and strategies to improve the superconducting properties of real materials.
For this, a systematic exchange of knowledge between different institutions, and the creation of common databases of experimental and ab-initio data seem to be of primary importance. The workshop has also evidenced that one of the key problems of the field is that of improving the description of magnetic fluctuations from first-principles, since spin fluctuations are likely to be the leading mechanism for high-T_c superconductivity.
All these problems require high computational power and development of efficient algorithms, therefore it is likely that computer power will become a key issue in the field in the next few years.
The participants have also agreed that it would be important to hold this meeting on a regular basis (every second year seems a reasonable time-frame), and to try and setup other initiatives to increase cooperations on a European ad international level.

Annex 4a: Programme of the meeting

Workshop Structure

	Monday 30	Tuesday 1	Wednesday 2	Thursday 3	Friday 4
	Chair: W. Pickett	Chair: I. Mazin	Chair: A. Carrington	Chair: R. Gonnelli	Chair: E.K.U. Gross
9:00	Arrival and Registration	M. Cohen: **DFT methods** and discussion	P. Canfield: **key experiments** and discussion	Hanke **strong correlation** and discussion	Closing Remarks
9:30					T. Takayama
10:00	Opening workshop				M. Aichhorn
10:30	D.J. Scalapino: **theory of superconductivity** and discussion	R. Gonnelli	Discussion	C. Franchini	Discussion
11:00		Discussion	R. Margine	Discussion	W. Pickett
11:30		M. Calandra	F. Giustino	A. Carrington	G. Giovannetti
12:00	S. Parkin	J. Zaanen	A. Linscheid	J. Annett	I. Mazin
12:30	Lunch break	Lunch break	Lunch break	Lunch break	Lunch break
13:00					
13:30					
	Char: D. Singh	Chair: S. Parkin	Chair: I. Zaanen	Chair: J. Annett	
14:00	Journal Club	G. Profeta	Discussion	A. Kolmogorov	
14:30		Discussion		C. Heil	Organizers Wrapping up and discussion
15:00				Discussion	
15:30	Coffee Break	I. Eremin	Coffee Break		
16:00	C. Giannetti	D. Singh	P. Hirschfeld: **weakly correlated models** and discussion	Coffee Break	Coffee Break
16:30	S. Curtarolo: **high throughput methods** and discussion	Coffee Break		Discussion	Discussion
17:00		Round Table			
17:30					

Annex 4b: Full list of speakers and participants

- Aichhorn Markus University of Technology Graz Austria
- Annett James University of Bristol United Kingdom
- Boeri Lilia ITP-CP Tu Graz Austria *
- Calandra Matteo CNRS and Université P. et M. Curie France
- Canfield Paul Iowa State University / Ames Lab United States
- Carrington Antony University of Bristol United Kingdom
- Cohen Marvin UC Berkeley United States
- Curtarolo Stefano Duke University United States
- Eremin Ilya Ruhr-Universität Bochum Germany
- Giannetti Claudio Università Cattolica Italy
- Giovannetti Gianluca CNR-IOM & SISSA Italy
- Giustino Feliciano University of Oxford United Kingdom
- Gonnelli Renato DISAT - Politecnico di Torino Italy
- Gross Eberhard MPI of Microstructure Physics Germany *
- Hanke Werner Universität Würzburg Germany
- Heil Christoph ITPCP TU Graz Austria
- Hirschfeld Peter U. Florida/U. Frankfurt Germany
- Kolmogorov Aleksey Binghamton University United States
- Linscheid Andreas MPI für Mikrostrukturphysik Germany
- Margine Elena Roxana Binghamton University - SUNY United States
- Marques Miguel ILM, CNRS and University of Lyon France *
- Mazin Igor NRL United States
- Parkin Stuart IBM Research - Almaden United States
- Pickett Warren UC Davis United States
- Profeta Gianni University of L'Aquila Italy
- Sanna Antonio Max Planck Institute Germany *
- Scalapino Douglas UCSB United States
- Singh David Oak Ridge National Laboratory United States
- Takayama Tomohiro Max Planck Institute for Solid State Res Germany
- Zaanen Jan LION Netherlands

All participants except those indicated with a * have contributed a talk.