

THE TASK IS,
NOT SO MUCH TO SEE
WHAT NO ONE HAS
YET SEEN;
BUT TO THINK
WHAT NOBODY HAS
YET THOUGHT,
ABOUT THAT WHICH
EVERYONE SEES.



INSIDE REPORTING ON 2002/03

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Pedro Miguel Echenique Landiribar President

DIPC started as an intellectual center with the principal aim of promoting and facilitating the development of basic and oriented research in materials science to the highest level.

WELCOME TO THE DIPC FOUNDATION

PRESENT AND FUTURE

The Donostia International Physics Center (DIPC) Foundation was created in 1999, as a fruit of foresighted collaborations between the Departments of Education and Industry of the Basque Government, the University of the Basque Country, the Provincial Authority of Gipuzkoa, the Town Hall of San Sebastian and the savings bank, Kutxa of San Sebastian and Gipuzkoa.

DIPC started as an intellectual center with the principal aim of promoting and facilitating the development of basic and oriented research in materials science to the highest level. DIPC has therefore been open and associated to the University of the Basque Country and an internationalization platform for basic science in the Basque Country in the field of materials science.

In order to meet these goals, in the first consolidation stage, three basic programs were established:

1. Visiting Researchers Program
2. International Workshops Program
3. General Science Communication Program

The aim of the **Visiting Researchers Program** was to attract the best scientists in the field of materials science. Thus, an interaction platform between researchers of high recognition from other countries and our researchers was established. From this platform, the emergence of new joint project proposals would not only be favored but the creation of an international network which allows for a better understanding and diffusion of our own scientific activity.

The **International Workshops Program** was intended to create new platforms for debate in which experts from different arenas but with common goals would contribute to the resolution of hot topics. Rather than adopting the ▶

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Juan Colmenero de León General Director

In this short period, DIPC has become a center of reference in basic research of Materials Physics.

In addition to DIPC scientific level, it is also gaining recognition internationally as a center of innovation, as other universities and research centers have recently shown interest in our model of operation.

► conventional format of a conference, informal meeting with a reduced number of invited scientists was preferred in order to provide plenty of free time for discussions.

Finally, the **General Science Communication Program** was intended to bring the world of science to the public. The social implication of this program is evident since a person will not be considered educated without some basic knowledge of scientific and technical issues.

After four years, we can say that the objectives we set from the start have been accomplished. In this short period, DIPC has become a center of reference in basic research of Materials Physics. The relevance is supported by the quality of the researchers who have visited the center, the international level of the workshops held and most of all, the importance of the scientific contributions derived from the research activity. For instance, during the period of the time of this report, 2002-03, 187 original papers have been

published in journals such as, Physical Review Letters (21 papers) and Physical Review (55 papers). This means that the contribution in 2002-03 from DIPC in these journals is in the order of 8% of the total contribution by Spanish institutions. This is quite an achievement for such a young institution.

It is also important to note the launching of the first stage of Fellows Guipuzkoa. This program, under the financial support of the Provincial Authority of Guipuzkoa, allows young scientists, mostly from the Basque Country, who have been working abroad, to return. DIPC acts as a "landing platform" by means of a five-year contract. ►

Juan Colmenero de León is Professor of Condensed Matter Physics at the University of the Basque Country. He obtained his PhD in Physics by the University of Navarra (1979). His research activities are Polymer Physics and Non-Crystalline Materials. He is a member of the Editorial Board of the Journals: Colloid & Polymer Science (Springer) and Journal of Polymer Science B, Polymer Physics (WILEY). He is also Chairman of the Selection Panel of the European Project "Jülich Neutrons for Europe" and Spanish representative at the Advisory Committee of the Institute Laue Langevin (ILL, Grenoble). He has been awarded the "Xabier María de Munibe" Prize in Science & Technology (1998) given by the Basque Parliament and the Euskadi Prize of Research in Science & Technology (2000) given by the Basque Government.



Alberto López Basaguren Secretary

We hope that the new computation center will become one of the basic pillars for future developments of scientific activity at DIPC through continuous updates in hardware.

The principal objective in this second stage of development is the creation of a critical mass of staff researchers at DIPC.

► In addition to DIPC scientific level, it is also gaining recognition internationally as a center of innovation, as other universities and research centers have recently shown interest in our model of operation.

Spurred by these remarkable results after our initial launching stage, we now face the challenge of developing DIPC into a powerful center for basic research. Along the same line, we can include the creation of our new in-house Computation Center. This center arose with the aim of becoming an international reference in complex computational physics and materials simulation. We hope that the center will become one of the basic pillars for future developments of scientific activity at DIPC through continuous updates in hardware.

The principal objective in this second stage of development is the creation of a critical mass of staff researchers at DIPC. The idea does not consist of repeating the schemes of other centers,

with permanent staff positions, but of habilitating medium term contract staff (one to three years) in numbers which would allow for the proper exploitation of existing know how and resources. In order to reach this objective, we have started a new postdoctoral and PhD contract grant program. These new programs, along with the established Fellows Guipuzkoa, and the external grant systems, will enable for the attainment of a critical mass of researchers based at DIPC.

The deployment of these programs also requires a substantial increase in the budget of the Foundation. In addition, new spaces will have to be made available, which will involve the refurbishment of the fourth building at the DIPC premises. ■

Alberto López Basaguren is Professor of constitutional law. He obtained his degree in political sciences from Universidad Complutense in Madrid and PhD from the University of the Basque Country (1990). He furthered his studies in Florence and Bologna (Italy). He continues his research in economic, constitutional and linguistic law and its integration in the European Community. He is formerly Secretary General of the University of the Basque Country.



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NEW SPACE

THE OPENING OF THE DIPC COMPUTATION CENTER

One of the priorities of Donostia International Physics Center is the development of basic research in materials science at the highest level. Within this line, DIPC relies on complex computational calculus and simulation methods as basic tools. The developments in this science advance towards complexity and towards multi-component, nano-structured and biological materials. It is widely accepted that modern computation and simulation methods, along with the future development of computers, will be indispensable in this field. DIPC intends to develop multi-scale calculation and simulation methods, which are appropriate for the study and modeling of materials. The scope of the fields covered ranges from the electronic and atomic scale (*"ab-initio"* methods) as well as molecular, nanometric and mesoscopic scales.

The first phase of the new DIPC Computation Center was inaugurated at DIPC in July 2003. The institute's own calculation center is connected to the general service of the University of the Basque Country (UPV/EHU) and is optimized for

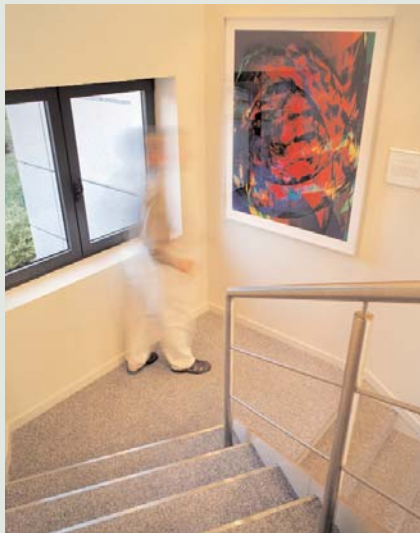


Patrons and board members examine the first installed units at the opening of the Computation Center.

From left to right: Joseba Jaureguizar, José Ramón Guridi, José Ignacio Telletxea, Juan Colmenero, Fernando Cossío, Jon Ramón Beloki, Alfredo Zalaia, and Alberto López Basaguren.

computational and simulation purposes in materials science. This center operates with an open layout, which will allow for new modern methods, such as intensive distributed and interconnection calculus to be carried out with other international computation facilities. This however will require the constant deployment of adequate up-to-date computational hardware. ■

The new DIPC Computation Center affords the opportunity for Basques and DIPC's visitors to access a facility with state-of-the-art calculating power.





The development of this center will require the constant deployment of adequate up-to-date computational hardware.

Patrons of the DIPC Foundation, from left to right: Juan Colmenero, Anjeles Iztueta, Pedro Miguel Echenique, Josu Jon Imaz and Alberto López Basaguren.



Odón Elorza, José Ignacio Telletxea, Fernando Cossio, Juan Colmenero and Félix Ares.

RESEARCH ACTIVITY

DIPC is dedicated to two main areas of research.

CONDENSED MATTER PHYSICS

The current activity —mainly theory and computational physics— is focussed on four different lines: Theory of Scanning Tunneling Microscopy, Interactions of ions with matter; Electronic response of surfaces, solids and nanostructures; Interaction of fast electrons and radiation with nanostructured materials. Moreover, a Nano-Physics Laboratory project is being developed in collaboration with a Technological Center of the Basque Country (Labein). Within these general areas, different recent topics can be identified:

Interaction of ions with matter

Phase effect in the stopping of ions in metals
Stopping of slow ions in insulators

Electronic response of surfaces, solids and nanostructures

Dynamics of electrons and holes in solids and at their surfaces
Electronic properties in finite and extended systems
Electronic structure and magnetic properties of nanowires

Interaction of fast electrons and radiation with nanostructured materials

Interaction of radiation and fast electrons with complex nanostructures (Smith-Purcell and microscopy based light emission induced by fast electrons)
Plasmon excitations in nanostructures
Photoemission from core and valence levels

POLYMERS AND NON-CRYSTALLINE MATERIALS

The current activities in this area are focussed on the general line: Molecular motions and relaxation processes in polymer materials and glass-forming systems. This is mainly an experimental approach by combining different techniques, in particular, neutron scattering, broadband dielectric spectroscopy and NMR. Moreover, we are also developing fully atomistic molecular dynamics simulations of polymer systems. Within this general area, we can identify the following recent topics of research:

Molecular motions and relaxation processes in polymer materials and glass- forming systems

*Dynamics of multicomponent
polymer systems*

Atomistic MD-Simulations in polymers

*Dynamics of glass-forming polymers and the
problem of the Glass Transition*

*Relationship between transport
properties and molecular mobility in polymeric
membranes*

*Microscopic understanding of relaxation
processes in engineering thermoplastics*