



XXIX Cursos de Verano
Uda Ikastaroak
XXII Cursos Europeos
Europar Ikastaroak

XXIX Cursos de Verano / XXIX. Uda Ikastaroak

XXII Cursos europeos / XXII. Europar Ikastaroak

Universidad del País Vasco / Euskal Herriko Unibertsitatea

Donostia - San Sebastián, 2010



4.1 SCHOOL

Summer School on Computational Materials Sciences (X)

Organisers:

Pedro Miguel Echenique Landiribar.

DIPC, Donostia-San Sebastián, the Basque Country.

Igor Abrikosov.

Linköping University, Sweden.

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Max Planck Institut für Eisenforschung, Germany.

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DIPC, Donostia-San Sebastián, the Basque Country.

Aims:

The Summer School on Computational Materials Sciences aims at the identification and promotion of the common elements developed in theoretical and computational studies of materials properties across materials types, metals, ceramics, materials for new energy technologies, electronic materials and minerals. To accomplish this goal, the School brings together leading experts from a wide spectrum of materials simulations including theory, modeling, and computation, engaged in the study of a broad range of materials properties. Several lectures will be devoted to experimental challenges in the field, and will be conducted by outstanding experimentalists within Materials Sciences.

Therefore, this School provides a forum for exposing young researchers and students to most recent state-of-the-art theoretical and computational developments in studying, understanding, and predicting the properties of materials. Also, the School encourages interdisciplinary contributions, such as between the fields of condensed matter physics and applied materials sciences, chemistry, metallurgy, etc.

The proposed conference is the third in the series of Schools organized successfully in collaboration between CECAM and Psi-k at Miramar Palace, San Sebastian, Spain. In 2007 the Psi-k Training Summer School "Ab initio Many Body Theory" attracted 108 students and 19 lecturers. In 2009 the Summer School on Simulation Approaches to Problems in Molecular and Cellular Biology is scheduled for 31 August-5 September.

Once again the emphasis of the School on Computational Materials Sciences will be on attracting scientists, students, and young researchers in the fields of basic science, e.g., electronic structure and related properties, assessing alloy phase diagrams, semiconductor physics, mineral science, and phenomenology. The emphasis on cross-fertilization of subject matter and the interdisciplinary character of the presentations make these meetings unique. The master classes scheduled during the School will give basic training in the use and understanding of state-of-the-art simulation tools.

The basic purpose of the present School is to continue to break down communication barriers across the various materials related disciplines and to foster, promote, and enhance a concerted and unified theoretical approach to study of materials properties. Therefore, this School is intended to help practitioners, both experimentalists and theorists who are involved in studying complex inorganic solids and materials, to obtain first-hand information from the leading experts in the respective field. This will enhance their own perspectives and horizons as well as those of their colleagues.

It is our vision that promoting such an integrated approach to materials science at the level of young researchers will have important and welcome consequences. It will provide a healthy

response to the present and rapidly changing situation in theory, where new and exciting areas of scientific inquiry become more and more evident. It may open the possibility to apply methods and techniques established in one field to a different one, thus opening the door for innovative funding proposals. The young materials scientist, metallurgist, solid state physicist, mineralogist, and chemist will clearly benefit from the School.

CECAM, Psi-k and Max-Planck-Institute für Eisenforschung, in collaboration with the Donostia International Physics Center (DIPC).

Special registration fee.

For further information, please, visit the website: http://dipc.ehu.es/ws_presentacion.php?id=53
Contact: cms10@ehu.es

Academic validity: 60 hours.

Official language: English.

European activity.

PROGRAM

June 28

- 9:00 h Basic class: "Intro to DFT"
J. NEUGÉBAUER.
Max-Planck-Institut. Düsseldorf. Germany.
- 10:30 h Coffee break
- 11:00 h Basic class: "KKR/CPA"
I. ABRIKOSOV.
Linköpings University. Linköping. Sweden.
- 12:30 h Lunch
- 15:15 h Intro talks/poster
- 16:00 h Break
- 16:15 h Intro talks/poster
- 17:30 h Coffee break
- 18:00 h Master class: "Using VASP for materials simulations"
S. SIMAK.
Linköpings University. Linköping. Sweden.

June 29

- 9:15 h Basic class: "Alloys / magnetism"
A. RUBAN.
Royal Institute of Technology (KTH). Stockholm. Sweden.
- 10:30 h Coffee break
- 11:00 h Basic class: "Cluster expansion"
M. ASTA.
University of California. Davis. California. USA.
- 12:30 h Lunch
- 15:15 h Special: "SMAs"
A. AYUELA.
DIPC and Unidad de Física de los Materiales, Centro Mixto CSIC-UPV/EHU, Basque Country.
- 16:00 h Break
- 16:15 h Intro talks/poster
- 17:30 h Coffee break
- 18:00 h Master class: "Effective cluster interactions"
A. RUBAN.
Royal Institute of Technology (KTH). Stockholm. Sweden.

June 30

- 9:15 h Basic class: "BOP"
R. DRAUTZ.
ICAMS. Ruhr-Universität Bochum. Germany.
- 10:30 h Coffee break
- 11:00 h Basic class: "Empirical potentials"
S. DUDAREV.
EURATOM/UKAEA Fusion Association. Oxfordshire. UK.
- 12:30 h Lunch
- 14:00 h ¿Walking?

July 1

- 9:00 h Basic class: "New functionals"
K. BURKE.
University of California. Irvine. California. USA.
- 10:30 h Coffee break

- 11:00 h Basic class: "DMFT"
A. GEORGES.
École Polytechnique. Paris. France.
- 12:30 h Lunch
- 15:00 h Basic class: "Point defects"
C. VAN DE WALLE.
University of California. Santa Barbara. California. USA.
- 16:30 h Break
- 16:40 h Special: "Impurity states"
H. RAEBIGER.
Yokohama National University. Yokohama. Japan.
- 17:30 h Coffee break
- 18: 00 h Master: "Defects"
K. BURKE.
University of California. Irvine. California. USA.
- 18:45 h Master: "Beyond DFT"
C. FREYSOLDT.
Max-Planck-Institut. Düsseldorf. Germany.

July 2

- 9:00 h Basic class: "Phonons/ meta-stable phases"
V. OZOLINS.
UCLA, USA.
- 10:30 h Coffee break
- 11:00 h Basic class: "Order N methods"
P. ORDEJON.
Centre d'Investigació en Nanociència i Nanotecnologia (CIN2). Barcelona.
- 12:30 h Lunch
- 15:30 h Special: "Hydrogen stor"
J.A. ALONSO.
University of Valladolid. Valladolid.
- 16:30 h Break
- 16:40 h Special: "Quasi particles"
P. RINKE.
Fritz Haber Institute. Berlin. Germany.
- 17:30 h Coffee break

18:00 h Master: “Order N DFT”
D. SANCHEZ-PORTAL.
Donostia International Physics Center (DIPC). CFM-UPV/EHU. Donostia-San Sebastián.

18:45 h Master: “Surf. Dynamics”
R. DIEZ-MUIÑO.
Donostia International Physics Center (DIPC). CFM-UPV/EHU. Donostia-San Sebastián.

July 3

9:00 h Basic class: “CALPHAD”
P. KORZHAVYI.
Royal Institute of Technology (KTH). Stockholm. Sweden.

10:30 h Coffee break

11:00 h Basic class: “Liquids”
D. ALFE
University College London. UCL. London. UK.

16:40 h Special: “Ab initio TD”
T. HICKEL.
Max-Planck-Institut. Düsseldorf. Germany.

17:30 h Coffee break

18:00 h Master class: “Thermo-dynamics”
B. GRABOWSKI.
Max-Planck-Institut. Düsseldorf. Germany.

Programa provisional - Behin behinekoa - Draft