

The Abdus Salam **International Centre for Theoretical Physics**





Workshop on "Advanced Oxide Interfaces" 9 - 12 May 2011

followed by the

ADGLASS General Meeting 13 May 2011

Miramare - Trieste, Italy

The Abdus Salam International Centre for Theoretical Physics (ICTP, Trieste, Italy) is organizing a Workshop on "Advanced Oxide Interfaces" to be held at the ICTP from 9 to 12 May 2011. The General Meeting for the members of the ADGLASS consortium will follow the Workshop on the 13 May 2011.

DESCRIPTION: Understanding the properties of oxide interfaces has widespread implications in materials science, engineering, electronics, and physics. Ceramic coatings used in modern structural glasses, oxide films used in smart fuel cells or in the basic components of advanced biomedical devices used in orthopedics and dentistry, all rely on the optimal performance of oxide interfaces in aggressive chemical environments. The mechanical and electronic properties of oxide interface are tightly connected to their atomistic structure, which is in turn the result of a complex interplay between the properties of the different phases involved (e.g., crystalline or glassy) and the chemical nature of the bonding between the relevant ionic species across the interface. Atomistic modeling plays a fundamental role in this area. It complements experimental efforts by providing an atomistic interpretation of the results. Moreover, modeling can be used as a guide in the design of new materials with enhanced properties, desirable for practical applications. The atomistic modeling of oxide interfaces requires chemical accuracy and at the same time must be able to treat large systems, up to several thousand atoms. It is thus an ideal playground for the development of atomistic methods capable of bridging length and time scales with "ab-initio" accuracy.

Topics of the Workshops include: structural and mechanical properties of oxide interfaces, classical potentials for oxide systems, DFT for oxides, the "Learn On The Fly" method, multiscale methods, spectroscopical methods, chemical methods, crack propagation experiments, technological applications of oxide interfaces.

The Workshop is organized in cooperation and with the co-sponsorship of the EU consortium ADGLASS (www.adglass.eu). The consortium focuses on two specific applications: adhesion of proteins at the interface between a glassy SiO₂ phase and a water solution, relevant to pharmaceutical applications; and the cohesion between a glassy SiO₂ phase and crystalline TiO₂ phases, relevant for applications in architectural glass and photovoltaic cells.

PARTICIPATION: Scientists and students from all countries that are members of the United Nations, UNESCO or IAEA may attend the workshop from 9 to 12 May 2011. Participation in the ADGLASS General Meeting is restricted to consortium members only. As the Workshop will be conducted in English, participants should have an adequate working knowledge of this language. Although, the main purpose of the Centre is to help research workers from developing countries, through a programme of training activities within a framework of international cooperation, a limited number of students and post-doctoral scientists from developed countries are also welcome to attend.

As a rule, travel and subsistence expenses of the participants should be borne by their home institution. Every effort should be made by candidates to secure support for their fare. However, very limited funds are available for partial support of some participants who are nationals of, and working in, a developing country, and who are not more than 45 years old. Such support is available only for those who attend the entire Workshop. There is no registration fee for attending this activity.

HOW TO APPLY FOR PARTICIPATION

An Online Application Form can be accessed through the Workshop website

http://agenda.ictp.it/smr.php?2236

Once in the website, comprehensive instructions will guide you step-by-step on how to fill out and submit the Application Form.

WORKSHOP SECRETARIAT:

Telephone: +39-040-2240346 Fax: +39-040-224163 E-mail: smr2236@ictp.it ICTP Home page: http://www.ictp.it/

in cooperation with and

co-sponsored by:

EU Consortium for Glass Interfaces

ORGANIZERS:

Lucio COLOMBI-CIACCHI (Bremen University, Germany)

Alessandro DE VITA (King's College London, U.K.)

> Hoger RÖHL (SCHOTT, Germany)

<u>LOCAL ORGANIZER:</u>

Sandro SCANDOLO (ICTP, Trieste, Italy)

TENTATIVE LIST OF SPEAKERS:

Noam BERNSTEIN (Naval Research Lab., Washington DC, U.S.A.)

> Lucio COLOMBI-CIACCHI (Bremen University, Germany)

Gabor CSANYI (Cambridge University, U.K.)

Alessandro DE VITA (King's College London, U.K.)

Michael MOSELER (Freiburg University, Germany)

Mike PAYNE (Cambridge University, U.K.)

> Hoger RÖHL (SCHOTT, Germany)

Dov SHERMAN (Technion, Haifa, Israel)

Paul TANGNEY (Imperial College, London, U.K.)

Deadline for Application:

27 FEBRUARY 2011