The Abdus Salam International Centre for Theoretical Physics

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United Nations Educational, Scientific and Cultural Organization

IAEA International Atomic Energy Agency

College on Multiscale Computational Modeling of Materials for Energy Applications

4 to 15 July 2016

(ICTP, Miramare, Trieste, Italy)

The Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy is organizing a ***College on Multiscale Computational Modeling of Materials for Energy Applications,*** to be held at ICTP, Trieste, Italy, ***4 to 15 July 2016.*** The event is being co-sponsored by ***INRS - Énergie Matériaux Télécommunications Research Centre,*** *Varennes, Canada,* ***ESF*** *- European Science Foundation and* ***Psi-K*** *Network.*

Nowadays, computational materials science has several challenges: 1) keep the accuracy of the model to appropriately obtain the physical properties of the materials; 2) integrate the methodologies available for the different time and length scales, ranging from electronic, atomistic to mesoscopic and continuum levels required to study some physical-chemical phenomena and 3) provide key information to be directly applied in the energy sector at an industrial level.

This College aims to bring a multiscale view of the materials modelling techniques for energy applications. More specifically, a multiscale methodology ranging from atomistic to mesoscopic and continuum methods will be presented with potential use of materials for industrial applications in: (i) fuel cells and catalysts, (ii) rechargeable batteries, (iii) solar energy conversion and solar fuels, (iv) semiconductors for light emitting technologies and (v) oil recovery techniques. It will also include general lectures on the socio economic impact related to the choice of energy technologies, experimental challenges and engineering challenges.

TOPICS COVERED:

- Big Picture Challenges
- Experimental Challenges
- Engineering Challenges
- Socio-Economic and Political Challenges
- Multiscale Computational Modeling of Materials
- Fuel Cells
- Batteries
- Enhanced Oil Recovery
- Nanostructured Materials for Energy Applications

The College is aimed at physicists and engineers, experts in energy applications, either carrying out research or working in the academic or industrial sector in the field, and with a background in computer simulations related to condensed matter physics, chemistry or materials science. Participants ***are encouraged to make a poster.*** If interested, kindly submit a short one-page abstract of the contribution (size A4), attached to the online application. As the event will be conducted in English, participants should have an adequate working knowledge of this language.

GRANTS

A limited number of grants are available to support travel and living expenses of selected participants, with priority given to participants working in a developing country and who are at the early stages of their career.

TO REQUEST PARTICIPATION:

Online Application Form can be accessed at the following activity website:

http://indico.ictp.it/event/7656/

Activity Secretariat: **E-mail: smr2874@ictp.it**
Telephone: +39-040-2240305 Telefax: +39-040-224163
ICTP Home Page: http://www.ictp.it

(Trieste, Decemberr 2015)

Co-sponsors:

INRS UNIVERSITÉ DE RECHERCHE RESEARCH UNIVERSITY

EUROPEAN SCIENCE FOUNDATION

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**** ICTP Organizers***

SPEAKERS:

Francesca BALETTO
(King's College, London, U.K.)
Edo BOEK
(Imperial College, U.K.)
Flavia CASSIOLA
(Shell, U.S.A.)
Maria CHAN
(Argonne National Lab., U.S.A.)
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(TUM, Germany)
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(Shell, India)
Sauro SUCCI
(CNR, Italy)

***to be confirmed**

DEADLINE to apply
(if financial support or visa required):

15 March 2016

DEADLINE to apply
(if NO financial support or visa required):

15 May 2016