## PASC16 Conference First Call for Abstracts for Minisymposia, Contributed Talks and Posters

# Materials Track: Computational Materials Science / Condensed Matter Physics/Chemistry

The **Platform for Advanced Scientific Computing** (PASC) is delighted to launch a **Call for Abstracts** for its next conference (PASC16) **cosponsored by the Association for Computing Machinery** (ACM). The Conference will be held **from June 8 to 10, 2016** at the *SwissTech Convention Center*, located on the campus of the École Polytechnique Fédérale de Lausanne (EPFL), Switzerland.

PASC16 Conference June 8-10, 2016 SwissTech Convention Center EPFL, Switzerland www.pasc16.org

The PASC Conference is a platform for interdisciplinary research across the areas of computational science, high-performance computing, and various domain sciences: Climate and Weather, Computer Science & Mathematics, Emerging Domains, Engineering, Life Sciences, Materials, Physics, and Solid Earth. PASC16 builds on a successful history with 350 international attendees in 2015. This year PASC continues to expand its program and welcomes your participation in a substantially larger event.

#### **TARGETED AUDIENCE**

The PASC16 Conference seeks to engage participants from academia, research labs and industry to address important issues in HPC and computational science. The PASC16 Conference is inviting researchers from diverse scientific backgrounds to promote interdisciplinary collaboration and exchange of expertise. The conference is an opportunity for researchers in branches of science that require computer modeling and high-performance simulations to discuss computational techniques and technologies.

### **PROGRAM**

The PASC16 Conference will offer five plenary lectures and one public lecture, complemented by minisymposia, contributed talks and poster sessions in its eight different scientific domains. It will also present for the first time a session dedicated to papers selected for publication in the ACM Digital Library (a call for papers will be distributed separately). Furthermore, CSCS will organize the **CSCS Update Meeting** targeting mainly our user community. The program will provide time for discussions within PASC scientific disciplines (inter-PASC Networks discussions), and an exhibition space.

#### **CONTRIBUTIONS**

Researchers from academia and industry are encouraged to participate and present their research in the form of **minisymposia**, **contributed talks** and/or **poster presentations**. PASC16 welcomes abstract submissions (1000 characters including spaces) in the following scientific fields:

- Climate and Weather
- Computer Science & Mathematics
- Emerging Domains (Special Topic: HPC and Big Data)
- Engineering
- Life Sciences
- Materials
- Physics
- Solid Earth

Contributions should be submitted using the online submission system. Guidelines regarding the submission process and access to the online submission system are available at: http://www.pasc16.org/submission/

#### FOCUS FOR THE MATERIALS TRACK

Over recent years, computer simulation has revolutionized the way we do materials science. Partly as a result of the exponential growth in available computer power, and partly due to advances in methods and algorithms that are able to take best advantage of high-end computing resources, computational simulations in materials science, condensed matter physics, and chemistry are now a fundamental complement to experiments.

Computer simulations enable experimental conditions to be recreated *in silico*, and can provide information and understanding that is difficult to resolve or access in an experiment. They also permit investigations that would be challenging or impossible, such as modelling materials in extreme environments, or examining the effect of subtle changes in structure and composition on the properties of a system.

The areas covered in this track include (but are not limited) to applications and development of methods for:

- Materials design and discovery
- Nanoscience and nanotechnology
- Materials for energy
- Functional or structural materials
- Minerals and high-pressure studies
- Molecular systems
- Catalysis and electrochemistry
- Biochemistry and biomaterials
- Strongly-correlated systems
- Magnetism and spintronics
- · Linear-scaling and multiscale modeling
- Electronic-structure methods

#### **SUBMISSION DEADLINES**

Minisymposia: January 12, 2016 Contributed Talks: March 2, 2016

Posters: April 3, 2016

#### **PROGRAM CHAIRS**

Jan Hesthaven, EPF Lausanne, Switzerland Nicola Marzari, EPF Lausanne, Switzerland Olaf Schenk, Università della Svizzera italiana, Switzerland Laurent Villard, EPF Lausanne, Switzerland

## SCIENTIFIC COMMITTEE TRACK CHAIRS

Climate & Weather: Peter Bauer, ECMWF, UK

Computer Science & Mathematics: Bastien Chopard, University of Geneva,

Switzerland

Emerging Domains: Costas Bekas, IBM Research, Zurich, Switzerland

**Engineering:** William Curtin, EPF Lausanne, Switzerland **Physics:** Lucio Mayer, University of Zurich, Switzerland

Materials: Gian-Marco Rignanese, Université Catholique de Louvain, Belgium

**Solid Earth:** Johan Robertsson, ETH Zurich, Switzerland **Life Sciences:** Felix Schürmann, EPF Lausanne, Switzerland

#### **SCIENTIFIC COMMITTEE FOR MATERIALS**

Gian-Marco Rignanese, Université Catholique de Louvain, Belgium (Chair) Michele Ceriotti, EPF Lausanne, Switzerland Marie-Pierre Gaigeot, Université d'Evry, France Arash Mostofi, Imperial College London, United Kingdom Alexandre Tkatchenko, Fritz Haber Institute Berlin, Germany

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