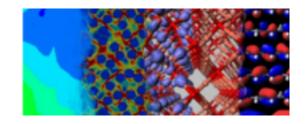
# International Workshop on Multiscale Modelling of Materials for Energy Conversion Applications



Thursday, November 8, 2012 - Friday, November 9, 2012
Athens, Greece

### **Invited Lectures**

A full list of contributions can be seen in the detailed view of the timetable and in the contribution list.

#### Grand challenges in multiscale modelling

Contributions:

Speaker: Prof. George FROUDAKIS

Title: Designing Nanoporous Materials for Hydrogen

Description

Speaker: Dr. Kurt STOKBRO

Title: ATK: An open platform for atomic-scale modeling

Description

#### Organic electronics, photovoltaics

Contributions:

Speaker: Dr. ANDRIENKO, Denis

Title: Challenges for in silico design of organic semiconductors for photovoltaic applications

Description

#### **Energy storage**

Contributions:

Speaker: Dr. Marie-Liesse DOUBLET

Title: Impact of the Interface Electrochemistry on the Li-Battery Performance: A first-step study

towards multi-scale modeling

Description

Speaker: Dr. Kourosh MALEK

Title: Modeling of Electrochemical Interfaces in Polymer Electrolyte Fuel Cells

Description

## Energy conversion: photovoltaics, dye-sensitized cells

Contributions:

Speaker: Dr. Filippo DE ANGELIS

Title: Modeling Dye-Sensitized Solar Cells from First Principles: Understanding the mechanism,

improving the efficiency

Description