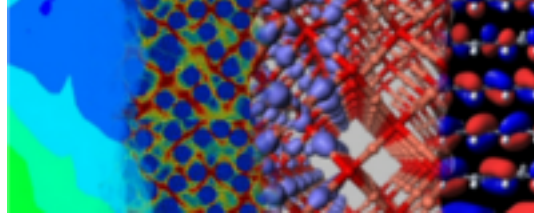


International Workshop on Multiscale Modelling of Materials for Energy Conversion Applications



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