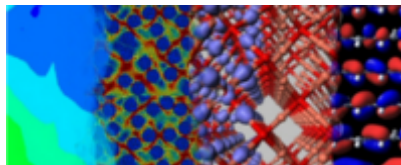


Session Program

Nov 8 - 9, 2012



International Workshop on Multiscale Modelling of Materials for Energy Conversion Applications

Session: Grand challenges in multiscale modelling (Click for details or select 'Detailed view')

Athens, Greece

The workshop will be held in a hotel in central Athens which will provide sufficient accommodation for all workshop participants. The hotel will be announced here by end of September and then you can book. In order to arrange for your travel we recommend to you to book a flight to Athens International Airport (Eleftherios Venizelos) from which the hotel will be accessed conveniently.

Thu, November 8

9:10 AM

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Session |

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Conveners: Marie-Liesse Doublet, Wolfgang Wenzel

09:10 – 09:55

ATK: An open platform for atomic-scale modeling

Speaker

Dr Kurt Stokbro

09:55 – 10:40

Designing Nanoporous Materials for Hydrogen

Speaker

Prof. George Froudakis

10:40 – 11:10

Coffee Break

11:10 – 11:35

Multiscale modelling on petascale supercomputers

Speaker

Andrew Emerson

11:35 – 12:00

A service-oriented approach for multiscale materials modelling and current challenges

Speaker

Dr Ivan Kondov

12:00 PM

2:00 PM

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Convener: Ivan Kondov

14:00 – 14:25

Multiscale Modelling with High Performance Architectures

Speaker

Prof. Wolfgang Wenzel

14:25 – 14:50

Divide-and-Conquer Learn-on-the-Fly: A Hybrid Quantum-Classical Approach for Simulating the Nanomechanical Properties of Metallic Systems

Speaker

Jacek Dziedzic

14:50 – 15:15

A virtual scientific computational environment for mobile devices

3:20 PM

Speaker
Haneol Cho