

International Workshop on Multiscale Modelling of Materials for Energy Conversion Applications

Thursday, November 8, 2012

Session: Grand challenges in multiscale modelling (Click for details or select 'Detailed view') (9:10 AM - 12:00 PM)

-Conveners: Marie-Liesse Doublet; Wolfgang Wenzel

| time | [id] title | presenter |
|----------|---|-------------------------|
| 9:10 AM | [4] ATK: An open platform for atomic-scale modeling | Dr STOKBRO, Kurt |
| 9:55 AM | [2] Designing Nanoporous Materials for Hydrogen | Prof. FROUDAKIS, George |
| 10:40 AM | Coffee Break | |
| 11:10 AM | [16] Multiscale modelling on petascale supercomputers | EMERSON, Andrew |
| 11:35 AM | [5] A service-oriented approach for multiscale materials modelling and current challenges | Dr KONDOV, Ivan |

Session: Grand challenges in multiscale modelling (Click for details or select 'Detailed view') (2:00 PM - 3:20 PM)

-Conveners: Ivan Kondov

| time | [id] title | presenter |
|---------|--|------------------------|
| 2:00 PM | [7] Multiscale Modelling with High Performance Architectures | Prof. WENZEL, Wolfgang |
| 2:25 PM | [17] Divide-and-Conquer Learn-on-the-Fly: A Hybrid Quantum-Classical Approach for Simulating the Nanomechanical Properties of Metallic Systems | DZIEDZIC, Jacek |
| 2:50 PM | [15] A virtual scientific computational environment for mobile devices | CHO, Haneol |