Venue: Hotel Ibis Alésia
Paris, France

Contact: Dr. Alexander Mavromaras
workshop2012@materialsdesign.com
+46 7 6893 5080 (Mobile)

Emergency Contact: Laetitia Cheguillaume
+33 6 98 39 16 96 (Mobile)

Agenda for Scientific Presentations on June 15th, 2012

Scientific presentations will discuss applications of the MedeA® software platform, theoretical developments and new software features and capabilities. The discussions on Friday provide an excellent opportunity for back-and-forth dialogue with our team, its senior scientists and developers. Materials Design will provide coffee throughout the day and lunch in the early afternoon.

08:10	Dr. Alexander Mavromaras, Materials Design Welcoming Remarks
08:15	Dr. Erich Wimmer, Materials Design *"The MedeA® software environment: Current capabilities and future directions"*
08:45	Dr. Clive Freeman, Materials Design *"Using MedeA® to compute materials properties in glasses, polymers, and other amorphous systems"*
09:30	Dr. Maria Entrialgo-Castaño and Dr. Xavier Rozanska, Materials Design *"Computing diffusion coefficients in amorphous systems – Application Examples and Demonstration"*
10:00	Coffee Break
10:30	Prof. Georg Kresse, University of Vienna *"What you should know about the selfinteraction error and large scale DFT simulations for Si_3N_4-xHy"*
11:30	Dr. Walter Wolf and Dr. René Windiks, Materials Design *"Metals and alloys: Mechanical properties, thermodynamics and transport from first-principles and embedding potentials"*
12:15	Lunch

MedeA® and Materials Design® are registered trademarks of Materials Design, Inc.

13:45	Dr. Volker Eyert and Dr. Mikael Christensen, Materials Design *"High precision electronic structure calculations for green applications – Overview and Application Examples"*
14:30	Dr. Philippe Ungerer, Materials Design *"State of the art and key challenges in fluid property prediction from classical Monte Carlo simulations"*
15:15	Coffee Break
15:45	Dr. Marianna Yiannourakou, Materials Design *"Predicting thermodynamic properties of fluid phases and sorption in solids using MedeA®-Gibbs – Application Example and Demonstration"*
16:15	Discussion
17:00	Adjourn

MedeA® and Materials Design® are registered trademarks of Materials Design, Inc.