The Research Computing and Cyberinfrastructure Group
and
The Material Simulation Center

PRESENTS

COMPUTATIONAL PREDICTION OF MATERIALS PROPERTIES WITH THE MEDEA SOFTWARE
presented by Hannes Schweiger

*Materials Design, Inc.*

Wednesday, June 23rd, 2010. 11:00 a.m. to 1:00 p.m.
Location: Room 141, Computer Building, Penn State University

**Introduction:**

This presentation will provide an overview of the capabilities of the MedeA software platform in predicting a wide range of material properties. Examples will include the effect of impurities and alloying elements on the strength of grain boundaries in metals, the computation of elastic moduli, the prediction of the electronic properties of materials and diffusion in solids. The MedeA platform makes it straightforward to build structures, launch and track a large number of calculations, analyze the results and to keep the computed data well organized. This is made possible by the integration of experimental and computed databases with high-performance computational codes such as VASP and LAMMPS within a flexible three-tier software architecture.

As part of the demonstration we will have the software installed and running on one of the RCC clusters.

**Registration:**

Please register by sending email to [mschelp@psu.edu](mailto:mschelp@psu.edu).

If there is a particular type of analysis you’d like to see demonstrated please let us know when you register.

Refreshments will be served.