



TMS 2012

141st Annual Meeting & Exhibition



March 11 – 15, 2012 • Walt Disney World Swan & Dolphin Resort • Orlando, Florida

Integrated Computational Materials Education

Sunday, March 11, 2012 • 8:30 a.m. – 4 p.m.

Member fee: **\$475**

Nonmember fee: **\$525**

Late Member fee: **\$550**

Late Nonmember fee: **\$600**

Course Description and Objectives:

Because computational techniques are becoming increasingly important in the design and development of new materials, there is a need to introduce undergraduate students to computational techniques as part of the core MSE curriculum. This short course is based on the Summer School for Integrated Computational Materials Education, which was developed to meet this need. We will present a set of materials that can be used in an existing undergraduate thermodynamics class using Thermo-Calc software, and an open-source code for Density-Functional-Theory (DFT) calculations. The short course includes lectures on the theory behind Thermo-Calc and DFT, a hands-on session on installing and using the software, and a lab session with computation-based problems. Participants will be provided with copies of materials and are encouraged to use them in their courses or assist their colleagues to implement them. Although the focus is on using Thermo-Calc and DFT codes in an educational setting, it is also appropriate for those interested in learning about the fundamentals of computational thermodynamics tools and first-principles energy methods for research and industrial applications.

Who should attend:

Professors, postdocs, and graduate students interested in integrating computational techniques into the undergraduate curriculum at their institutions; anyone interested in learning about the fundamentals of computational thermodynamics tools.

Instructors:

Larry K. Aagesen and **Katsuyo Thornton**

Department of Materials Science and Engineering
University of Michigan

Paul Mason

Thermo-Calc Software Inc.

Mark Asta

Department of Materials Science and Engineering
University of California, Berkeley

Short Courses