



Materials Simulation & Engineering

Summer School

“ Fundamentals of Thermodynamic Modelling of Materials ”

INSTN Saclay, July 2-6, 2012

- Use of computational techniques for design of superalloys **Roger Reed**, Birmingham University, UK
- Introduction to First Principles calculations **Philippe Baranek**, EDF, France
- Thermodynamics from First Principles **Roberto Dovesi**, Torino University, Italy
- Lattice dynamics of extended systems from density functional perturbation theory **Stefano Baroni**, SISSA, Italy
- Principles of Force Fields methods **Constantin Meis**, CEA - INSTN, France
- Thermodynamics from Force Fields **Julian Gale**, Curtin University, Australia
- Principles of Monte Carlo calculations **Frederic Soisson**, CEA Saclay, France
- Thermodynamic models **Bo Sundman**, CEA-INSTN, France
- Thermodynamic assessments **Bo Sundman**, CEA-INSTN, France
- Experimental data for assessments **Jean-Marc Joubert**, ICMPE, CNRS, France
- Extrapolations of thermodynamic properties **Suzana G. Fries**, Ruhr Univ., Germany
- Ab-initio calculations for compounds and solutions **Pavel Korzhavyi**, MSE, KTH, Sweden
- Diffusion from atomistic methods **Julian Gale**, Curtin University, Australia
- Multi-component diffusion **Lars Höglund**, MSE, KTH Sweden
- The Phase Field methods **Alphonse Finel**, ONERA, France
- Applications of Phase Field simulations **Markus Apel**, ACCESS, Germany
- Magnetic models **Pavel Korzhavyi**, MSE, KTH Sweden
- Modelling liquids from First Principles **Mark Asta**, Univ. of California Berkeley, USA
- Models for very high pressures **Michel Jacobs**, TU Clausthal, Germany

Multiple Computer Sessions with Relevant Softwares

Organizers:

Bo SUNDMAN, KTH, Sweden & CEA-INSTN, France
Constantin MEIS, CEA-INSTN, France
Julian GALE, Curtin University, Australia

Registration deadline: May 25, 2012

Registration and Information : Marie Noelle Claude
marie-noelle.claude@cea.fr (+33 1 69 08 50 40)

