

**WORKSHOP “FROM FIRST PRINCIPLES TO MULTI-SCALE MODELING OF MATERIALS”**

Time	Friday May 27 (Intercontinental)	Monday May 30 (Everest)	Tuesday May 31 (Everest and PUC-RIO)	Wednesday June 1 (Everest)
	CALPHAD Conference	FIRST PRINCIPLES AND THE CALPHAD METHOD	THERMODYNAMIC MODELLING- DATABASES AND SOFTWARE	KINETICS AND MICROSTRUCTURE PREDICTION
09:00- 10:30		Igor Abrikosov: Solution model and magnetism in first principle calculations	09:00-10:00 Bo Sundman: Assessment fundamentals in the CALPHAD method.  10:15-11:15 Sergei Decterov : Modeling oxide solutions - Quasi-chemical model and extrapolation to higher order systems.	Jim Warren: An overview of the fundamental and challenges of the application of phase field
10:45-12:15		Patrice Turchi: Predictions from Ab Initio Quantum Mechanics and Impact on Thermodynamic Assessment	11:15-12:45 Ursula Kattner: Quality assurance concepts in assessments and database construction	Bernd Böttger: Phase field modeling of technically important alloys
12:15-12:30			Morning discussion	Morning discussion
12:30 – 14:30		LUNCH	LUNCH	12:45-14:30 LUNCH
14:25	FIRST PRINCIPLES AND THE CALPHAD METHOD Welcome remarks by Prof Fernado Rizzo	FIRST PRINCIPLES AND THE CALPHAD METHOD	THERMODYNAMIC MODELLING- DATABASES AND SOFTWARE	SOFTWARES AND DATABASES
14:30- 15:30	Juan Sanchez: Overview of the cluster expansion method	Mauro Palumbo: "First- principles thermodynamic calculations in the harmonic and quasi-harmonic approximations using Quantum Espresso"	Hands on work on Simple Assessments and Database,	Bo Sundman: Open codes and the possible future of CALPHAD software
15:45- 16:45	Jörg Neugebauer: Overview of fundamentals of first principle calculation methods	THERMODYNAMIC MODELLING- DATABASES AND SOFTWARE Suzana Fries: The connection between solid state physics and the CALPHAD method	Hands on calculations with Quantum Espresso”	Suzana Fries: The experience with open databases and the integration of several sources of data in databases
16:45- 17:30	Discussion	Discussion		Discussion and Closing remarks by Prof Rizzo